

Computational Fluid Dynamics and Fire Modeling

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Fall 2001

References

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Nomenclature

ρ	density (kg/m ³)
$\mathbf{u} = (u, v, w)$	velocity (m/s)
$\boldsymbol{\omega} = \text{curl} \mathbf{u}$	vorticity (1/s)
$\mathbf{x} = (x, y, z)$	position (m)
$\mathbf{g} = (0, 0, -9.81)$	acceleration of gravity (m/s ²)
T	temperature (°C or K)
Y_i	mass fraction of i th species
Z	mixture fraction
D_i	diffusion coefficient of i th species (m ² /s)
\dot{W}_i'''	production rate of i th species (kg/m ³ /s)
p	pressure (Pa or atm)
μ	dynamic viscosity (kg/m s)
$\nu = \mu/\rho$	kinematic viscosity (m ² /s)
k	thermal conductivity (J/m s K)
c_p	specific heat, constant pressure (J/kg K)
c_v	specific heat, constant volume (J/kg K)
$\mathcal{R} = c_p - c_v$	gas constant (J/kg K)
$\gamma = c_p/c_v$	ratio of specific heats
e	internal energy per unit mass (J/kg)
$E = e + \mathbf{u} ^2/2$	total energy per unit mass (J/kg)
$h = e + p/\rho$	enthalpy (J/kg)
\dot{q}'''	heat source (W/m ³)

Notation

Gradient of a scalar field $\phi(x, y, z)$

$$\text{grad } \phi \equiv \nabla \phi = \left(\frac{\partial \phi}{\partial x}, \frac{\partial \phi}{\partial y}, \frac{\partial \phi}{\partial z} \right)$$

Dot Product of two vectors $\mathbf{f} = (f_1, f_2, f_3)$ and $\mathbf{g} = (g_1, g_2, g_3)$

$$\mathbf{f} \cdot \mathbf{g} = f_1 g_1 + f_2 g_2 + f_3 g_3$$

Velocity magnitude

$$|\mathbf{u}|^2 \equiv \mathbf{u} \cdot \mathbf{u} = u^2 + v^2 + w^2$$

Divergence of Velocity

$$\text{div } \mathbf{u} \equiv \nabla \cdot \mathbf{u} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}$$

Curl of Velocity (Vorticity)

$$\text{curl } \mathbf{u} \equiv \nabla \times \mathbf{u} \equiv \boldsymbol{\omega} = \left(\frac{\partial w}{\partial y} - \frac{\partial v}{\partial z}, \frac{\partial u}{\partial z} - \frac{\partial w}{\partial x}, \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right)$$

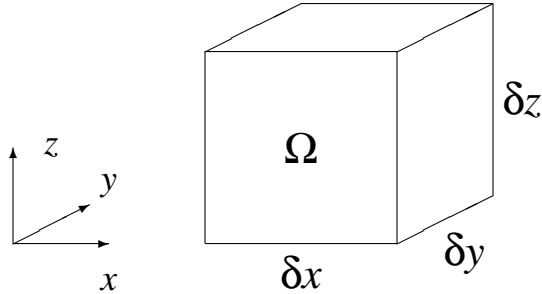
Second Rank Tensor

$$\boldsymbol{\tau} \equiv \tau_{ij} = \begin{pmatrix} \tau_{11} & \tau_{12} & \tau_{13} \\ \tau_{21} & \tau_{22} & \tau_{23} \\ \tau_{31} & \tau_{32} & \tau_{33} \end{pmatrix}$$

Tensor Divergence

$$\begin{aligned} \nabla \cdot (\mathbf{uu}) \equiv \text{div} (\mathbf{uu}) &= \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) \begin{pmatrix} u \\ v \\ w \end{pmatrix} (u, v, w) \\ &= \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) \begin{pmatrix} u^2 & uv & uw \\ vu & v^2 & vw \\ wu & wv & w^2 \end{pmatrix} \\ &= \left(\frac{\partial u^2}{\partial x} + \frac{\partial uv}{\partial y} + \frac{\partial uw}{\partial z}, \dots, \dots \right) \end{aligned}$$

Conservation of Mass



Fixed Control Volume Ω

Boundary denoted by $\partial\Omega$

Assume that the average density within Ω is $\rho_c(t)$. The mass contained within Ω is then $\rho_c \delta x \delta y \delta z$. The mass flowing in from the right (east) is $-u_e \rho_e \delta y \delta z$, the mass from the left (west) is $u_w \rho_w \delta y \delta z$, the mass from the back (north) is $-v_n \rho_n \delta x \delta z$, *etc.* Conservation of mass is expressed

$$\frac{d\rho_c}{dt} \delta x \delta y \delta z = -u_e \rho_e \delta y \delta z + u_w \rho_w \delta y \delta z - v_n \rho_n \delta x \delta z + \dots$$

Multiplying and dividing the terms on the RHS by δx , δy and δz , respectively, yields

$$\frac{d\rho_c}{dt} \delta x \delta y \delta z = -\frac{u_e \rho_e - u_w \rho_w}{\delta x} \delta x \delta y \delta z - \frac{v_n \rho_n - v_s \rho_s}{\delta y} \delta x \delta y \delta z - \frac{w_t \rho_t - w_b \rho_b}{\delta z} \delta x \delta y \delta z$$

More formally, the integral form of the Mass Conservation Equation is

$$\frac{d}{dt} \int_{\Omega} \rho dV = - \int_{\partial\Omega} \rho \mathbf{u} \cdot d\mathbf{S}$$

where $dV = dx dy dz$ and $d\mathbf{S} = \mathbf{n} dA$. Using the Divergence Theorem

$$\int_{\Omega} \nabla \cdot \mathbf{F} dV = \int_{\partial\Omega} \mathbf{F} \cdot d\mathbf{S}$$

the integral form can be written

$$\int_{\Omega} \frac{\partial \rho}{\partial t} dV = - \int_{\Omega} \nabla \cdot \rho \mathbf{u} dV$$

and the control volume can be made infinitesimally small, yielding

$$\boxed{\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0}$$

the conservation form of the equation. Introducing the material derivative

$$\frac{D(\cdot)}{Dt} = \frac{\partial(\cdot)}{\partial t} + \mathbf{u} \cdot \nabla(\cdot)$$

the equation can be written in “non-conservative form”

$$\boxed{\frac{D\rho}{Dt} + \rho(\nabla \cdot \mathbf{u}) = 0}$$

Note that if the density does not change, then $\nabla \cdot \mathbf{u} = 0$ and the fluid is incompressible.

For future reference, note that for a given scalar quantity $\phi(x, y, z, t)$

$$\frac{\partial \rho \phi}{\partial t} + \nabla \cdot \rho \mathbf{u} \phi \equiv \rho \frac{D\phi}{Dt}$$

because of the mass conservation equation. It is often convenient to write the transport equations in either of these forms.

Conservation of Species

If the fluid consists of a mixture of species, it is necessary to solve transport equations for each species. These equations have the form

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot \rho Y_i \mathbf{u} = \nabla \cdot \rho D_i \nabla Y_i + \dot{W}_i'''$$

where Y_i is the mass fraction of the i th species, D_i is the diffusion coefficient of species i into the mixture, and \dot{W}_i''' is the production rate of the species i . The constraint on the equations is that

$$\sum_{i=0}^N Y_i = 1 \quad ; \quad \sum_{i=0}^N \rho D_i \nabla Y_i = 0 \quad ; \quad \sum_{i=0}^N \dot{W}_i''' = 0$$

where there are $N + 1$ species in the mixture. Summing all the species equations together yields the mass conservation equation. Thus, one can solve $N + 1$ species equations or N species equations plus the mass conservation equation.

Conservation of Momentum

This is Newton's Second Law of Motion (Force = Mass \times Acceleration). Consider the component of momentum in the x -direction, ρu

$$\frac{d}{dt} \int_{\Omega} \rho u dV + \int_{\partial\Omega} \rho u \mathbf{u} \cdot d\mathbf{S} = \int_{\partial\Omega} -p \mathbf{i} \cdot d\mathbf{S} + \int_{\partial\Omega} (\boldsymbol{\tau} \cdot \mathbf{i}) \cdot d\mathbf{S}$$

where \mathbf{i} is the unit vector in the x direction and the viscous stress tensor of a Newtonian fluid is given as

$$\boldsymbol{\tau} \equiv \tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right) \quad ; \quad \delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

or

$$\boldsymbol{\tau} = \mu \begin{pmatrix} 2\frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} & \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \\ \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} & 2\frac{\partial v}{\partial y} & \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \\ \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} & \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} & 2\frac{\partial w}{\partial z} \end{pmatrix} - \frac{2}{3}\mu \begin{pmatrix} \nabla \cdot \mathbf{u} & 0 & 0 \\ 0 & \nabla \cdot \mathbf{u} & 0 \\ 0 & 0 & \nabla \cdot \mathbf{u} \end{pmatrix}$$

As with the mass conservation equation, the control volume can be shrunk to zero, and the resulting equation is

$$\frac{\partial \rho u}{\partial t} + \nabla \cdot \rho u \mathbf{u} = -\nabla \cdot p \mathbf{i} + \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{i})$$

After expansion of the terms the equation is

$$\begin{aligned} \frac{\partial \rho u}{\partial t} &+ \frac{\partial \rho u^2}{\partial x} + \frac{\partial \rho uv}{\partial y} + \frac{\partial \rho uw}{\partial z} = -\frac{\partial p}{\partial x} \\ &+ \frac{\partial}{\partial x} \left[\frac{2}{3}\mu \left(2\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} - \frac{\partial w}{\partial z} \right) \right] + \frac{\partial}{\partial y} \left[\mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] + \frac{\partial}{\partial z} \left[\mu \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \right] \end{aligned}$$

If the fluid is incompressible and the coefficient of viscosity is constant, this equation simplifies

$$\rho \frac{Du}{Dt} \equiv \rho \left(\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} \right) = -\frac{\partial p}{\partial x} + \mu \nabla^2 u$$

The vector form of the momentum equation is

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot \rho \mathbf{u} \mathbf{u} = -\nabla p + \rho \mathbf{g} + \nabla \cdot \boldsymbol{\tau}$$

or in non-conservation form

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \rho \mathbf{g} + \nabla \cdot \boldsymbol{\tau}$$

$$\frac{\text{mass}}{\text{volume}} \times \text{acceleration} = \frac{\text{force}}{\text{volume}}$$

Conservation of Energy

This is the First Law of Thermodynamics (Increase in energy of the control volume Ω is equal to the heat added minus the work done by expansion).

$$\begin{aligned} \frac{d}{dt} \int_{\Omega} \rho E dV + \int_{\partial\Omega} \rho E \mathbf{u} \cdot d\mathbf{S} &= \int_{\Omega} \dot{q}''' dV + \sum_{i=0}^N \int_{\partial\Omega} h_i \rho D_i \nabla Y_i \cdot d\mathbf{S} \\ &+ \int_{\partial\Omega} k \nabla T \cdot d\mathbf{S} + \int_{\partial\Omega} -p \mathbf{u} \cdot d\mathbf{S} + \int_{\partial\Omega} (\boldsymbol{\tau} \cdot \mathbf{u}) \cdot d\mathbf{S} + \int_{\Omega} \rho \mathbf{g} \cdot \mathbf{u} dV - \int_{\partial\Omega} \mathbf{q}_r \cdot d\mathbf{S} \end{aligned}$$

where $E = e + |\mathbf{u}|^2/2$ (internal + kinetic energy per unit mass). Rewrite in difference form:

$$\begin{aligned} \rho \frac{DE}{Dt} \equiv \rho \frac{De}{Dt} + \rho \frac{D(|\mathbf{u}|^2/2)}{Dt} &= \dot{q}''' + \sum_{i=0}^N \nabla \cdot h_i \rho D_i \nabla Y_i \\ &+ \nabla \cdot k \nabla T - \nabla \cdot p \mathbf{u} + \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{u}) + \rho \mathbf{g} \cdot \mathbf{u} - \nabla \cdot \mathbf{q}_r \end{aligned}$$

Using the momentum conservation equation

$$\rho \frac{D(|\mathbf{u}|^2/2)}{Dt} \equiv \rho \frac{D\mathbf{u}}{Dt} \cdot \mathbf{u} = -\nabla p \cdot \mathbf{u} + \rho \mathbf{g} \cdot \mathbf{u} + (\nabla \cdot \boldsymbol{\tau}) \cdot \mathbf{u}$$

write the energy equation as

$$\rho \frac{De}{Dt} + p(\nabla \cdot \mathbf{u}) = \dot{q}''' + \sum_{i=0}^N \nabla \cdot h_i \rho D_i \nabla Y_i + \nabla \cdot k \nabla T + \Phi - \nabla \cdot \mathbf{q}_r$$

where

$$\Phi \equiv \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{u}) - (\nabla \cdot \boldsymbol{\tau}) \cdot \mathbf{u} = \mu \left[2 \left(\frac{\partial u}{\partial x} \right)^2 + 2 \left(\frac{\partial v}{\partial y} \right)^2 + 2 \left(\frac{\partial w}{\partial z} \right)^2 + \right. \\ \left. \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right)^2 + \left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right)^2 + \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right)^2 - \frac{2}{3} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right)^2 \right]$$

Use the definition of enthalpy $h = e + p/\rho$ and rewrite

$$\rho \frac{Dh}{Dt} - \frac{Dp}{Dt} = \dot{q}''' + \sum_{i=0}^N \nabla \cdot h_i \rho D_i \nabla Y_i + \nabla \cdot k \nabla T + \Phi - \nabla \cdot \mathbf{q}_r$$

Equation of State

The gas can be assumed a Perfect Gas

$$p = \mathcal{R} \rho T \sum_{i=0}^N Y_i / M_i$$

Assuming that the specific heat of each species is independent of temperature, kinetic theory yields

$$c_{p,i} = \frac{2 + \nu_i}{2} \frac{\mathcal{R}}{M_i} = \frac{\gamma_i}{\gamma_i - 1} \frac{\mathcal{R}}{M_i}$$

where ν_i is the number of internal degrees of freedom of the molecules of the i th species. For diatomic molecules, $\nu = 5$ and $\gamma = c_p / c_v = 7/5$. Assuming all molecules in the mixture are diatomic and using the fact that the enthalpy of the mixture can be written

$$h = \sum_{i=0}^N h_i Y_i = T \sum_{i=0}^N c_{p,i} Y_i$$

the Equation of State can be simplified

$$p = \frac{\gamma - 1}{\gamma} \rho h$$

Basic Conservation Equations for Single Species

Conservation of Mass

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0$$

Conservation of Momentum

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot \rho \mathbf{u} \mathbf{u} = -\nabla p + \rho \mathbf{g} + \nabla \cdot \boldsymbol{\tau}$$

Conservation of Energy

$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot \rho h \mathbf{u} = \frac{Dp}{Dt} + \dot{q}''' + \nabla \cdot k \nabla T$$

Equation of State

$$p = \mathcal{R} \rho T$$

What are the unknowns? Density ρ ; Velocity Components u, v, w ; Enthalpy h , Pressure p

What needs to be provided? \dot{q}''' , the fire; $\boldsymbol{\tau}$, the (turbulent) viscous stresses, $\nabla \cdot k \nabla T$, thermal conductivity

Low Mach Number Form of Navier-Stokes Equations (Rehm and Baum)

Decompose pressure into average background pressure plus the hydrodynamic pressure plus a perturbation

$$p(x, y, z, t) = p_0 - \rho_\infty g(z - z_0) + \tilde{p}(x, y, z, t)$$

Mass Conservation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0$$

Momentum Conservation

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot \rho \mathbf{u} \mathbf{u} = -\nabla \tilde{p} + (\rho - \rho_\infty) \mathbf{g} + \nabla \cdot \boldsymbol{\tau}$$

Pressure Equation (Divergence of Momentum Equation)

$$\nabla \cdot \frac{\nabla \tilde{p}}{\rho} = -\frac{\partial(\nabla \cdot \mathbf{u})}{\partial t} + \dots \quad ; \quad \nabla \cdot \mathbf{u} = \frac{\gamma - 1}{\gamma p_0} (\dot{q}''' + \nabla \cdot k \nabla T)$$

Equation of State

$$p_0 = \mathcal{R} \rho T$$

Finite Difference Approximations

Recall from Calculus the Taylor series expansion of a function of one variable:

$$f(x + \delta x) = f(x) + \delta x \frac{df(x)}{dx} + \frac{\delta x^2}{2!} \frac{d^2 f(x)}{dx^2} + \dots + \frac{\delta x^n}{n!} \frac{d^n f(x)}{dx^n} + O(\delta x^{n+1})$$

The Taylor series expansion can be applied to a function of more than one independent variable. Consider a function of one time and one space variable:

$$\begin{array}{ll} \text{Time} & u(x, t + \delta t) = u(x, t) + \delta t \frac{\partial u}{\partial t}(x, t) + \frac{\delta t^2}{2} \frac{\partial^2 u}{\partial t^2}(x, t) + O(\delta t^3) \\ \text{Space} & u(x + \delta x, t) = u(x, t) + \delta x \frac{\partial u}{\partial x}(x, t) + \frac{\delta x^2}{2} \frac{\partial^2 u}{\partial x^2}(x, t) + O(\delta x^3) \end{array}$$

Assume $u(x, t)$ defined over the region $0 \leq x \leq L$ and $0 \leq t \leq \infty$. Divide the interval $[0, L]$ into I uniformly spaced cells of length $\delta x = L/I$, and let $u_i^n \equiv u(i\delta x, n\delta t)$ where δt is the size of a time step. Now the above expressions become

$$\begin{array}{ll} \text{Time} & u_i^{n+1} = u_i^n + \delta t \left(\frac{\partial u}{\partial t} \right)_i^n + \frac{\delta t^2}{2} \left(\frac{\partial^2 u}{\partial t^2} \right)_i^n + O(\delta t^3) \\ \text{Space} & u_{i+1}^n = u_i^n + \delta x \left(\frac{\partial u}{\partial x} \right)_i^n + \frac{\delta x^2}{2} \left(\frac{\partial^2 u}{\partial x^2} \right)_i^n + O(\delta x^3) \end{array}$$

which can be used to make approximations of partial derivatives, for example

$$\left(\frac{\partial u}{\partial t} \right)_i^n = \frac{u_i^{n+1} - u_i^n}{\delta t} + O(\delta t)$$

$$\begin{aligned}
\left(\frac{\partial u}{\partial x}\right)_i^n &= \frac{u_{i+1}^n - u_{i-1}^n}{2\delta x} + O(\delta x^2) \\
\left(\frac{\partial^2 u}{\partial x^2}\right)_i^n &= \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\delta x^2} + O(\delta x^2) \\
\left(\frac{\partial^3 u}{\partial x^3}\right)_i^n &= \frac{u_{i+2}^n - 2u_{i+1}^n + 2u_{i-1}^n - u_{i-2}^n}{2\delta x^3} + O(\delta x^2) \\
\left(\frac{\partial u}{\partial x}\right)_i^n &= \frac{-u_{i+2}^n + 8u_{i+1}^n - 8u_{i-1}^n + u_{i-2}^n}{12\delta x} + O(\delta x^4) \\
\left(\frac{\partial u}{\partial x}\right)_i^n &= \frac{3u_i^n - 4u_{i-1}^n + u_{i-2}^n}{2\delta x} + O(\delta x^2)
\end{aligned}$$

Model Problem: Burgers Equation

Consider the PDE

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2} \quad (1)$$

where $u(x, t)$ is defined for $0 \leq x \leq 1$ with initial conditions

$$u(x, 0) = f(x)$$

and boundary conditions

$$u(0, t) = 1 \quad ; \quad u(1, t) = 0$$

How does one solve this problem numerically?

Step 1. Divide the interval $[0, 1]$ into I uniformly spaced cells of length $\delta x = 1/I$, and let $u_i^n \equiv u(i\delta x, n\delta t)$ where δt is the size of a time step.

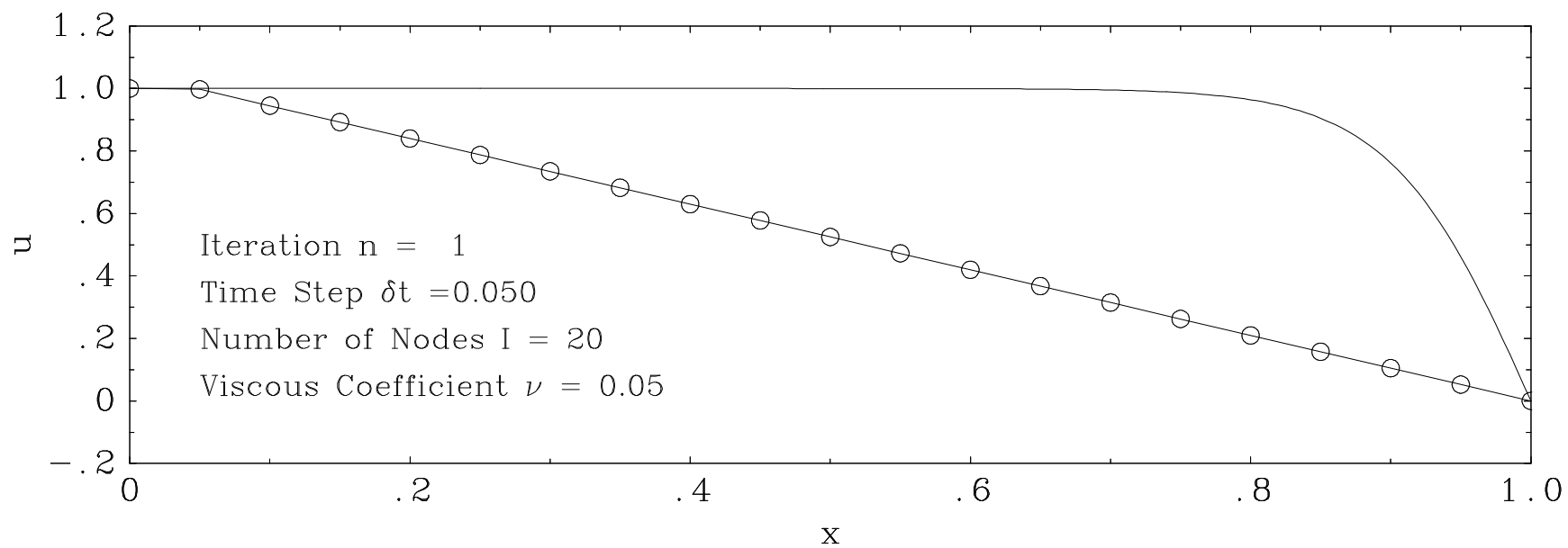
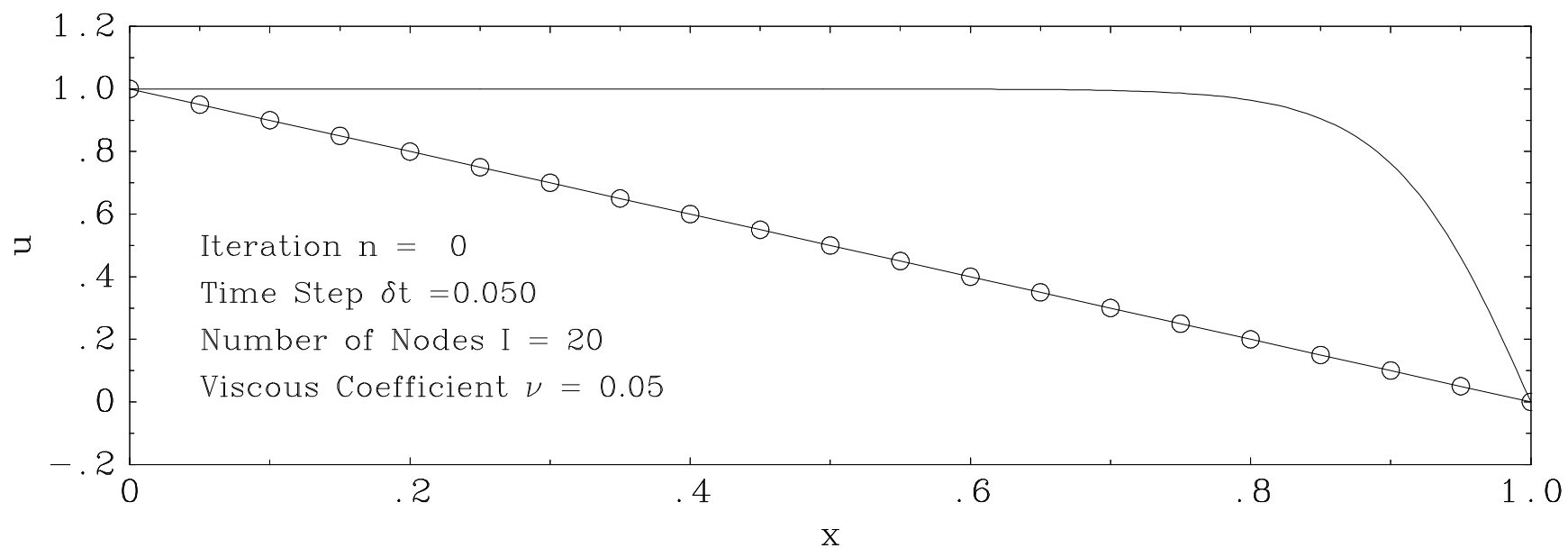
Step 2. Choose a discretization of Eq. (1) at each node i . One of the simplest discretizations is

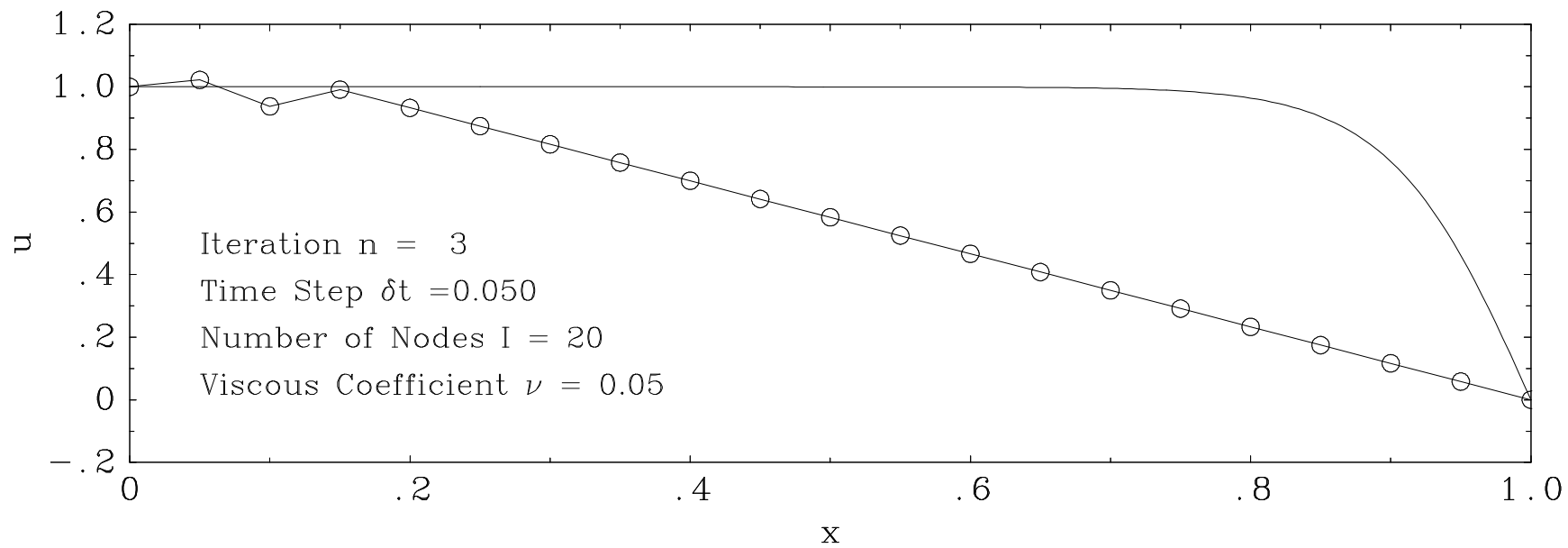
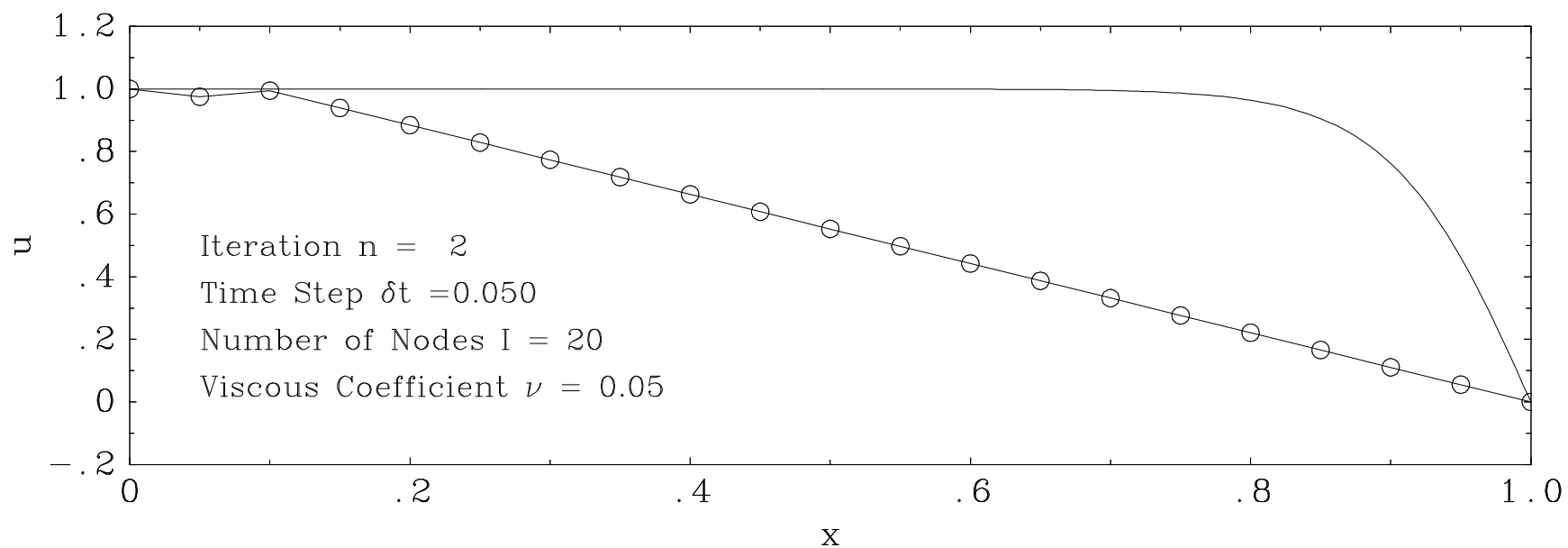
$$\frac{u_i^{n+1} - u_i^n}{\delta t} + u_i^n \frac{u_{i+1}^n - u_{i-1}^n}{2\delta x} = \nu \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\delta x^2}$$

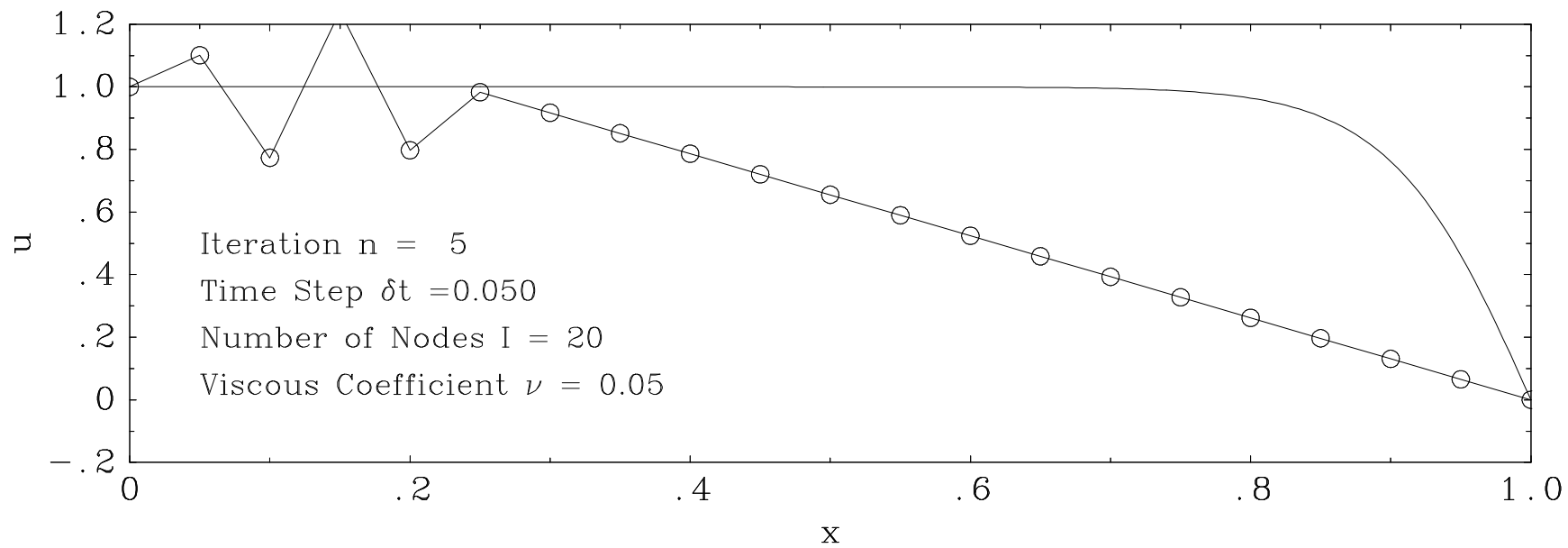
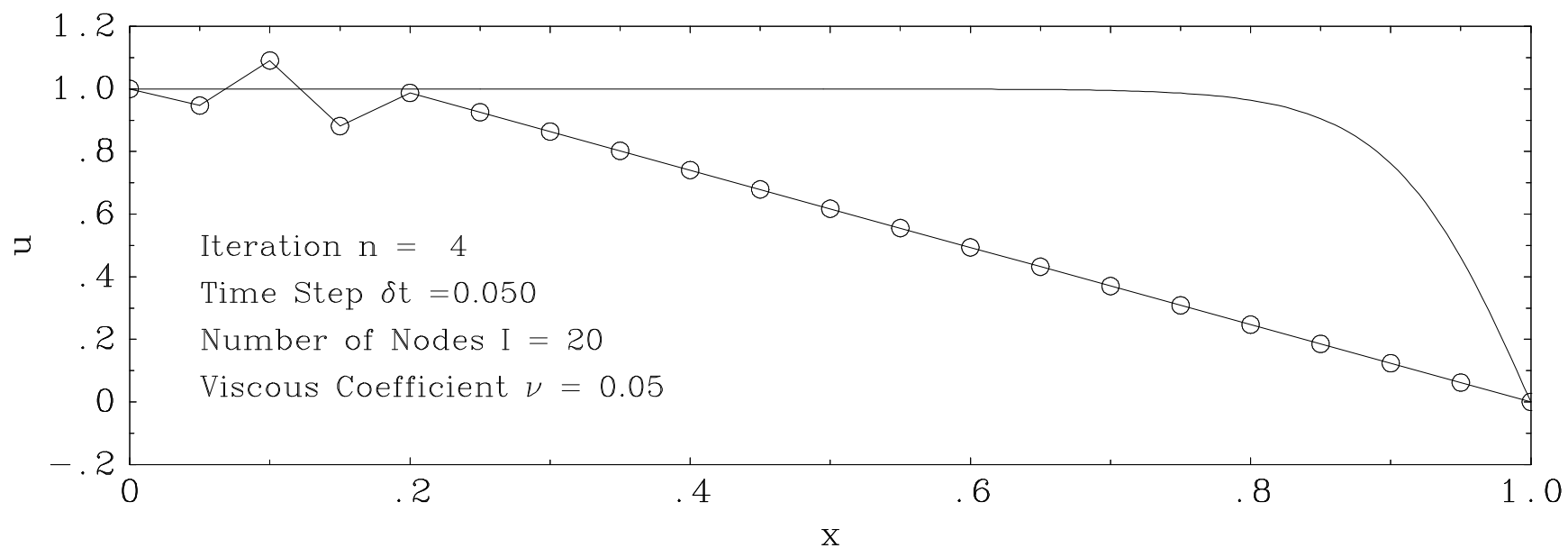
with initial condition $u_i^0 = f_i$ and boundary conditions $u_0^n = 1$ and $u_I^n = 0$.

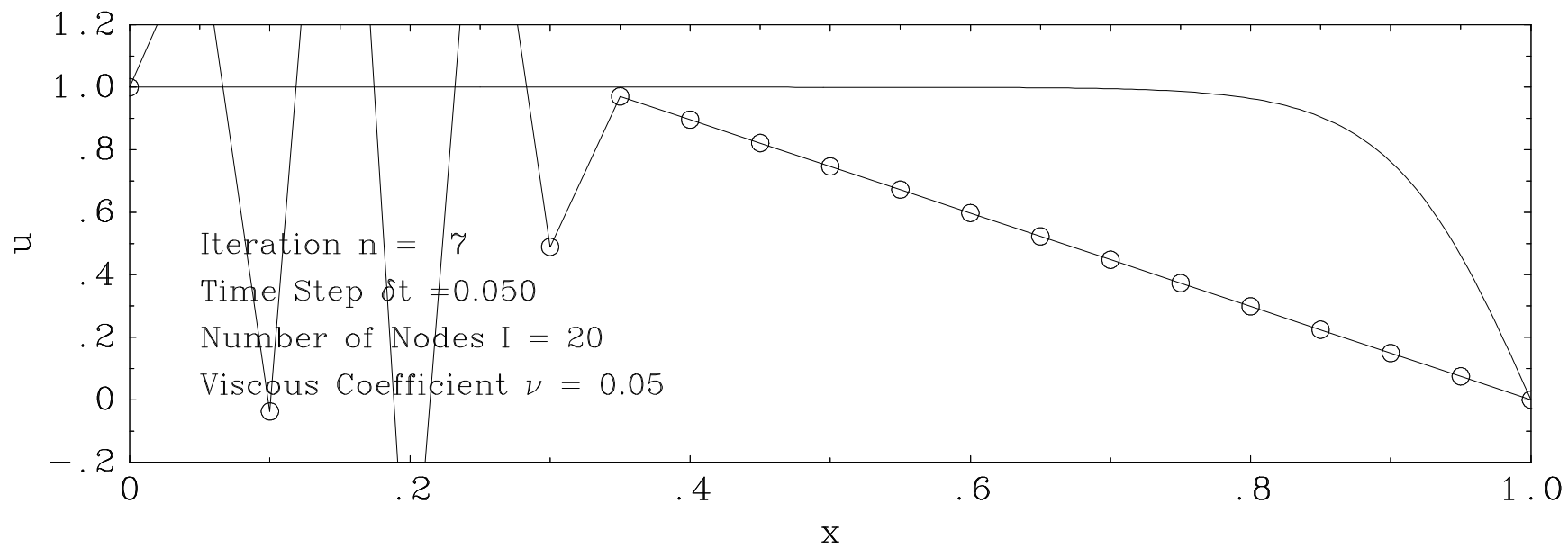
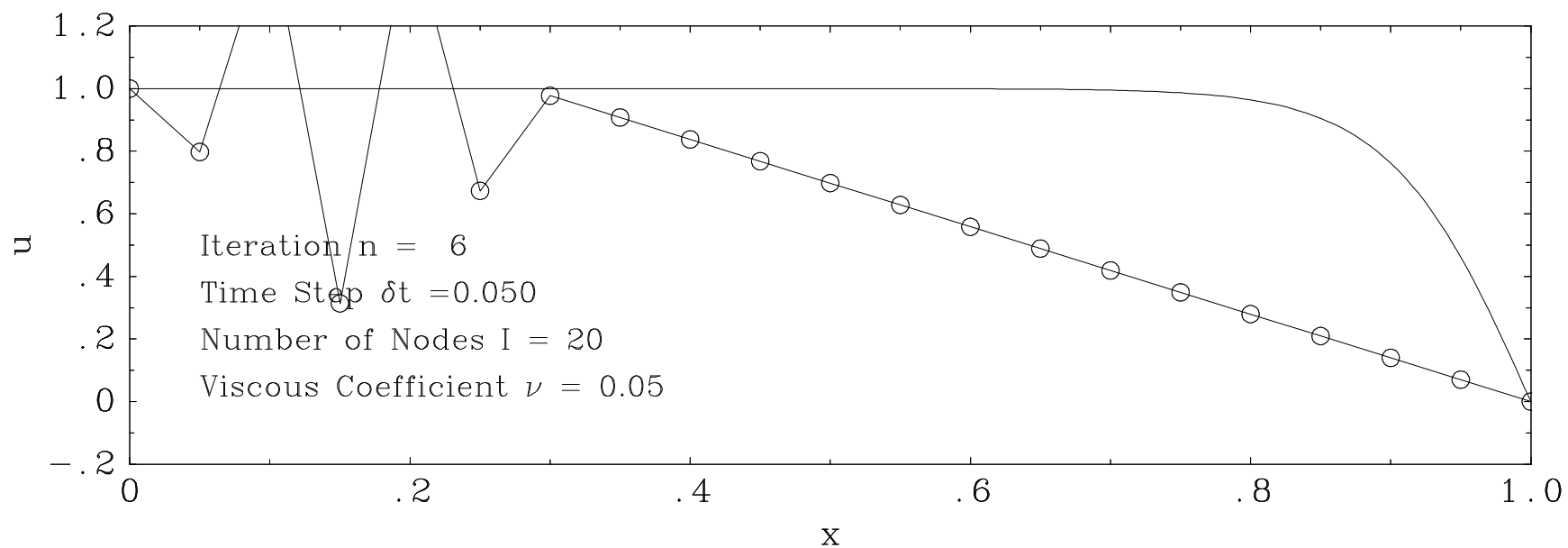
Step 3. Compute

$$u_i^{n+1} = u_i^n - \delta t \left[u_i^n \frac{u_{i+1}^n - u_{i-1}^n}{2\delta x} - \nu \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\delta x^2} \right]$$









What happened? To find out, ask what equation is *really* being solved.

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \left(v - \frac{u^2 \delta t}{2} \right) \frac{\partial^2 u}{\partial x^2} + \frac{u \delta x^2}{3} \left(\frac{3v \delta t}{\delta x^2} - \frac{u \delta t}{\delta x} - \frac{1}{2} \right) \frac{\partial^3 u}{\partial t^3} + \dots$$

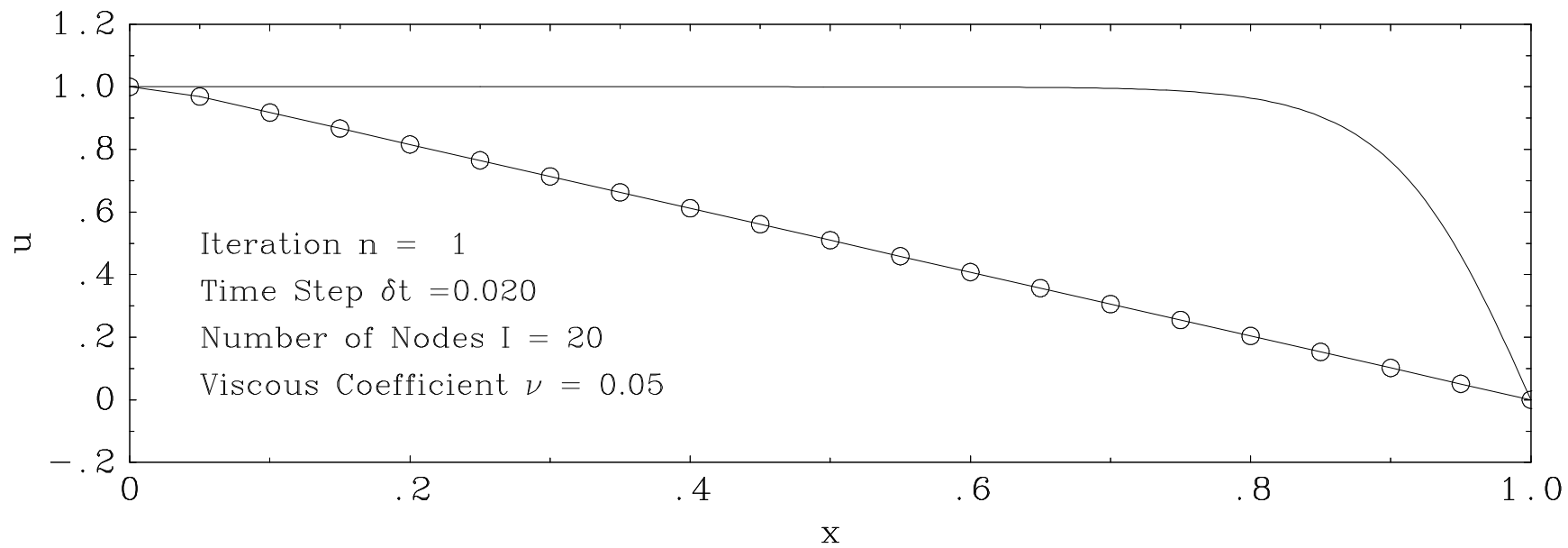
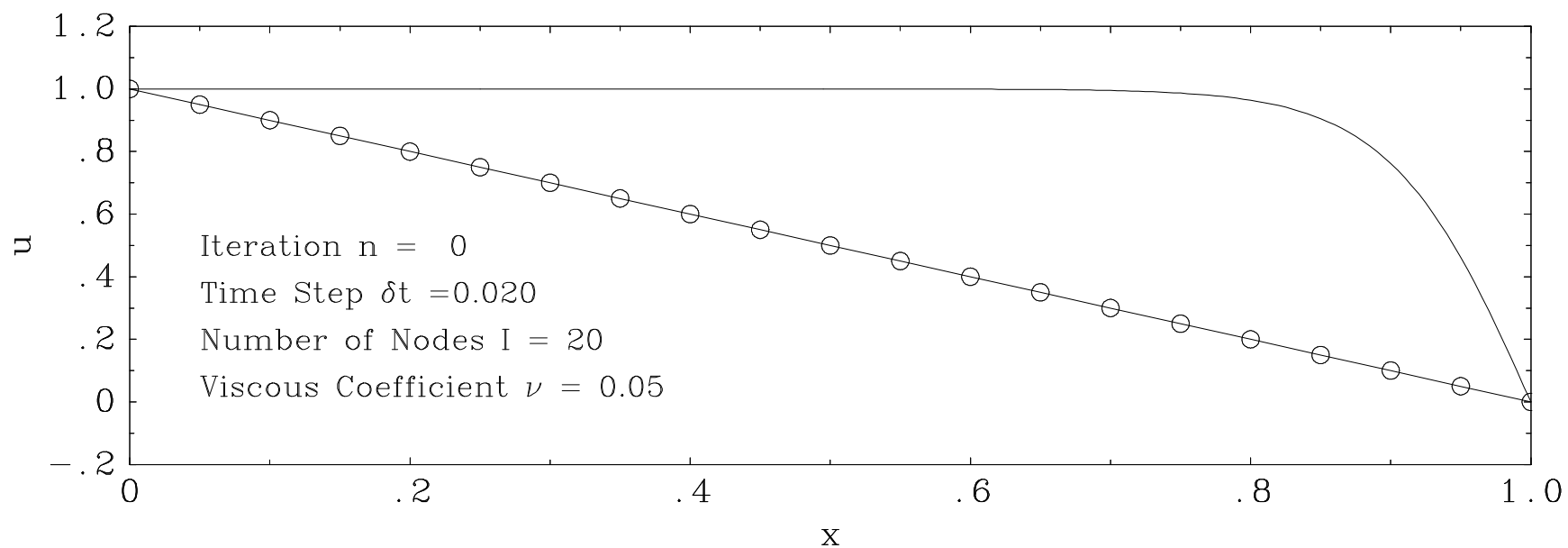
To avoid disaster, the time step size needs to be restricted according to

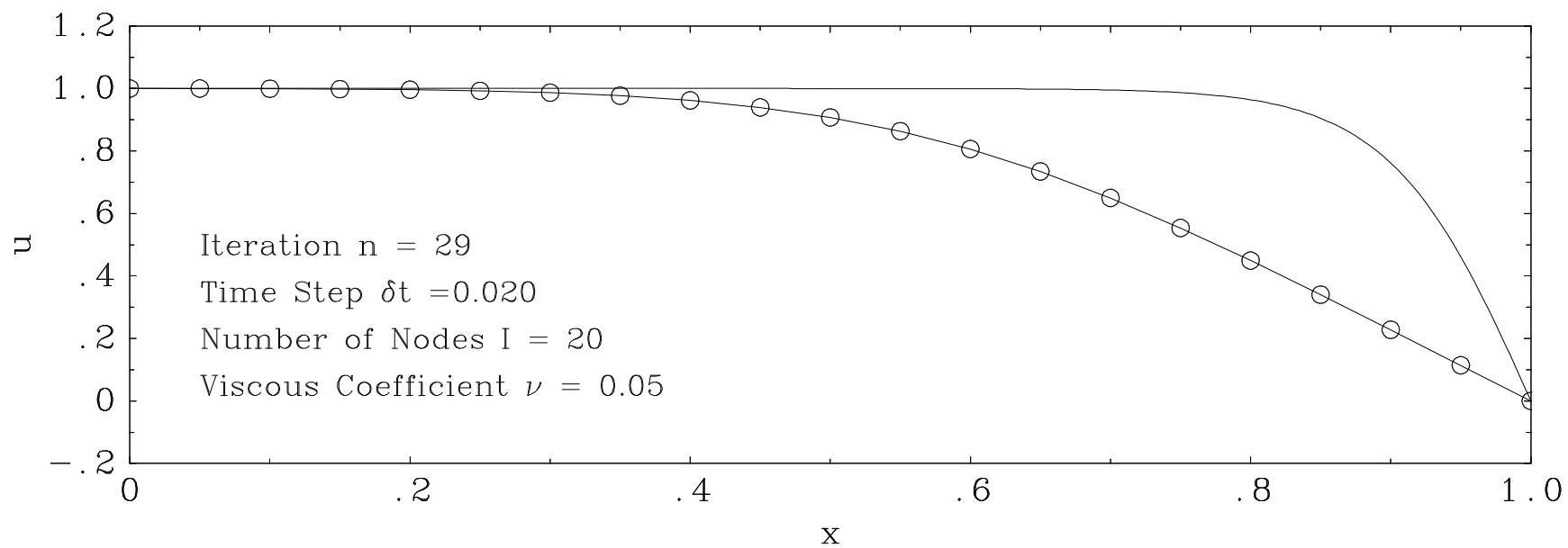
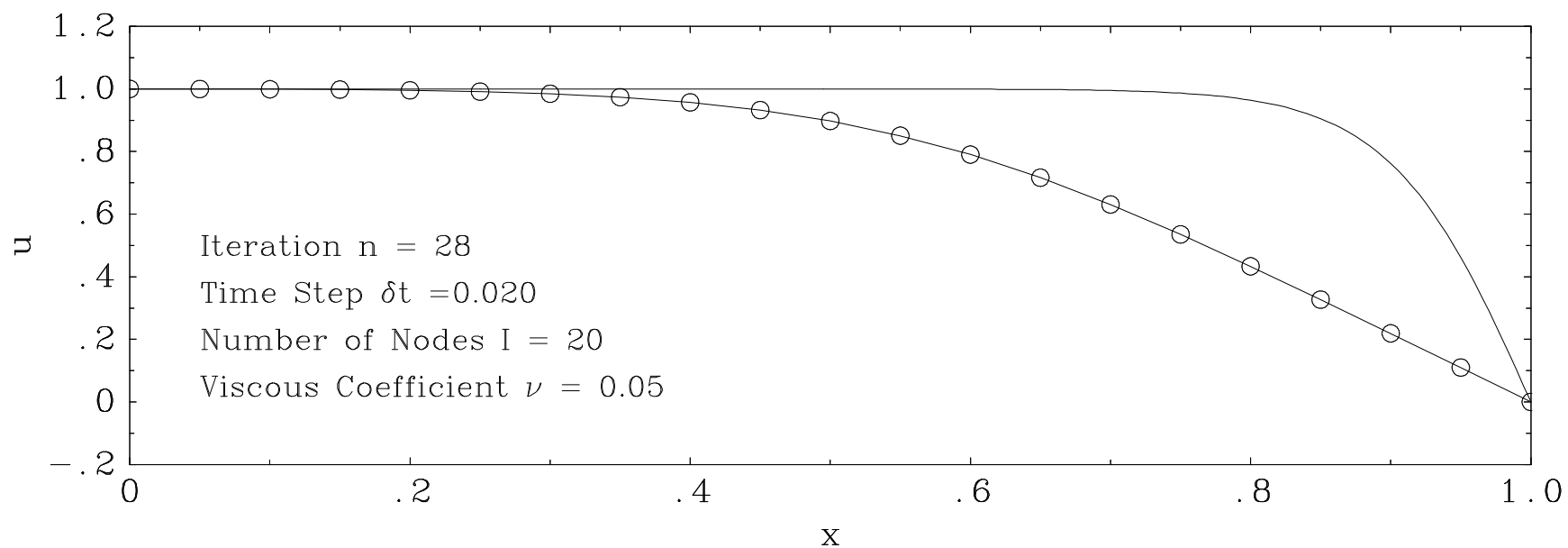
$$\delta t < \frac{\delta x^2}{2v} \quad \text{and} \quad \delta t < \frac{2v}{u^2}$$

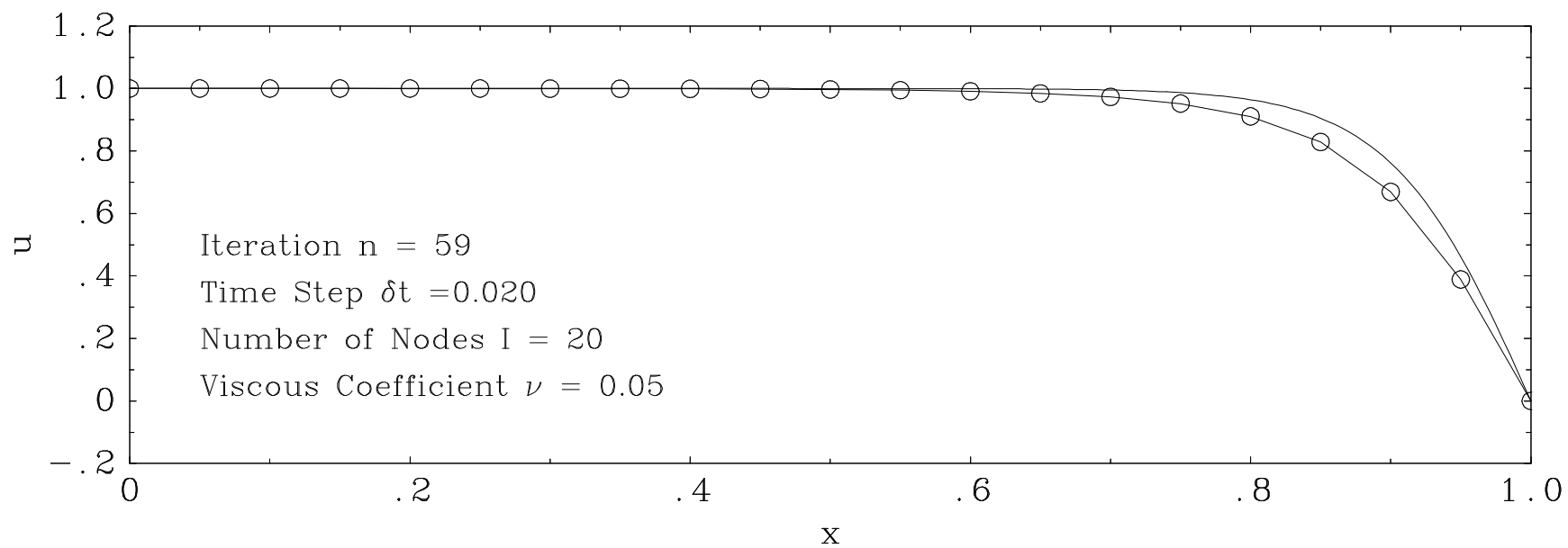
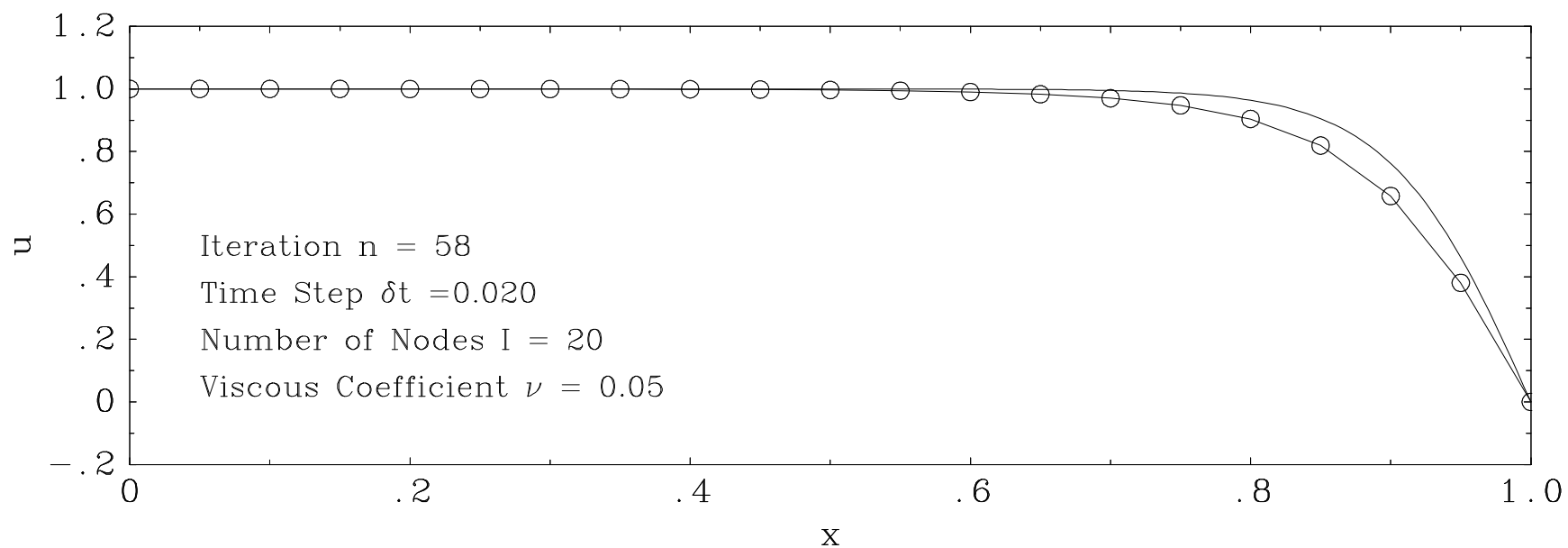
More often, these restrictions are written

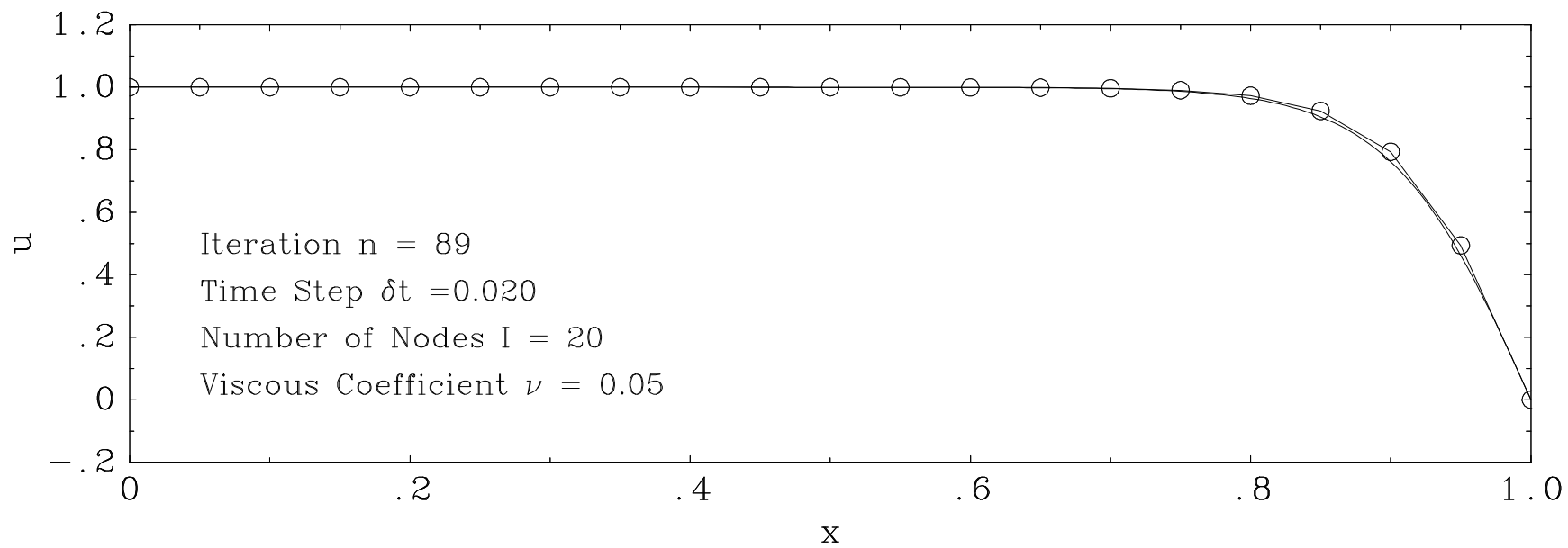
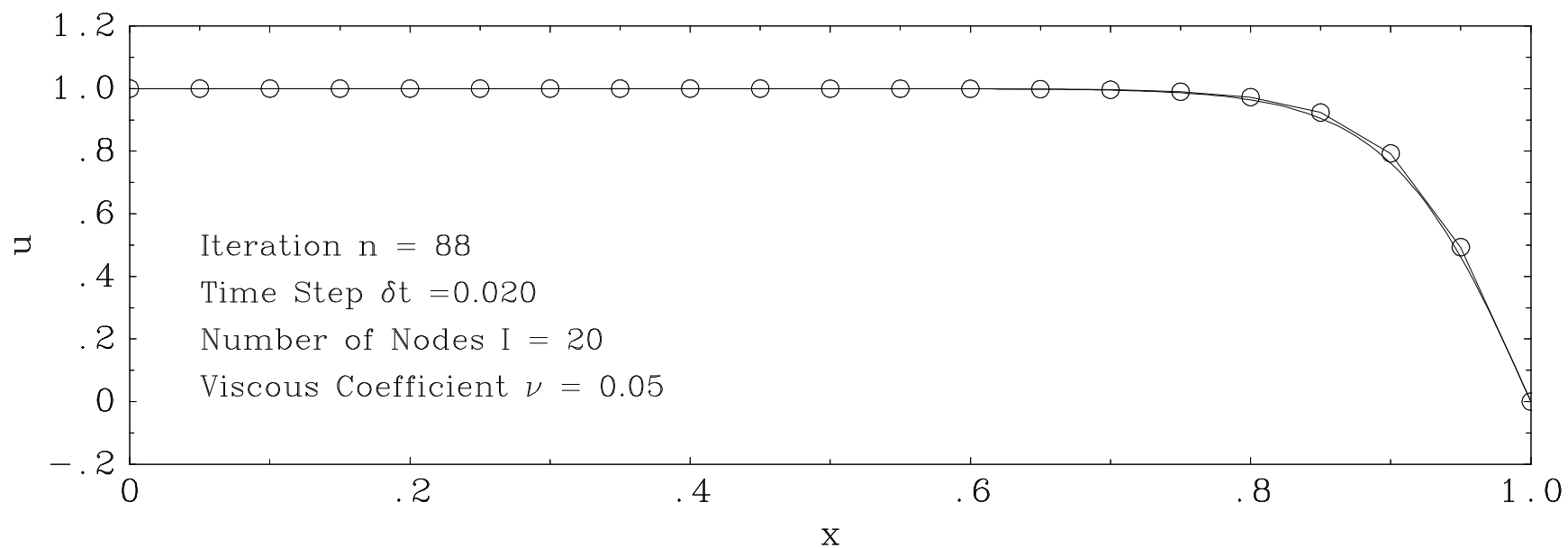
$$\delta t < \frac{\delta x^2}{2v} \quad \text{and} \quad \delta t < \frac{\delta x}{u}$$

and they apply to a lot of different schemes. The second restriction is known as the CFL condition (Courant, Friedrichs, Lewy, 1928).









An alternative discretization scheme is

$$\frac{u_i^{n+1} - u_i^n}{\delta t} + u_i^n \frac{u_i^n - u_{i-1}^n}{\delta x} = v \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\delta x^2}$$

with the same initial and boundary conditions as before. The equation that is being solved now is

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \left[v \left(1 + \frac{u \delta x}{2v} \right) - \frac{u^2 \delta t}{2} \right] \frac{\partial^2 u}{\partial x^2} + \dots$$

As long as

$$\delta t < \frac{\delta x}{u}$$

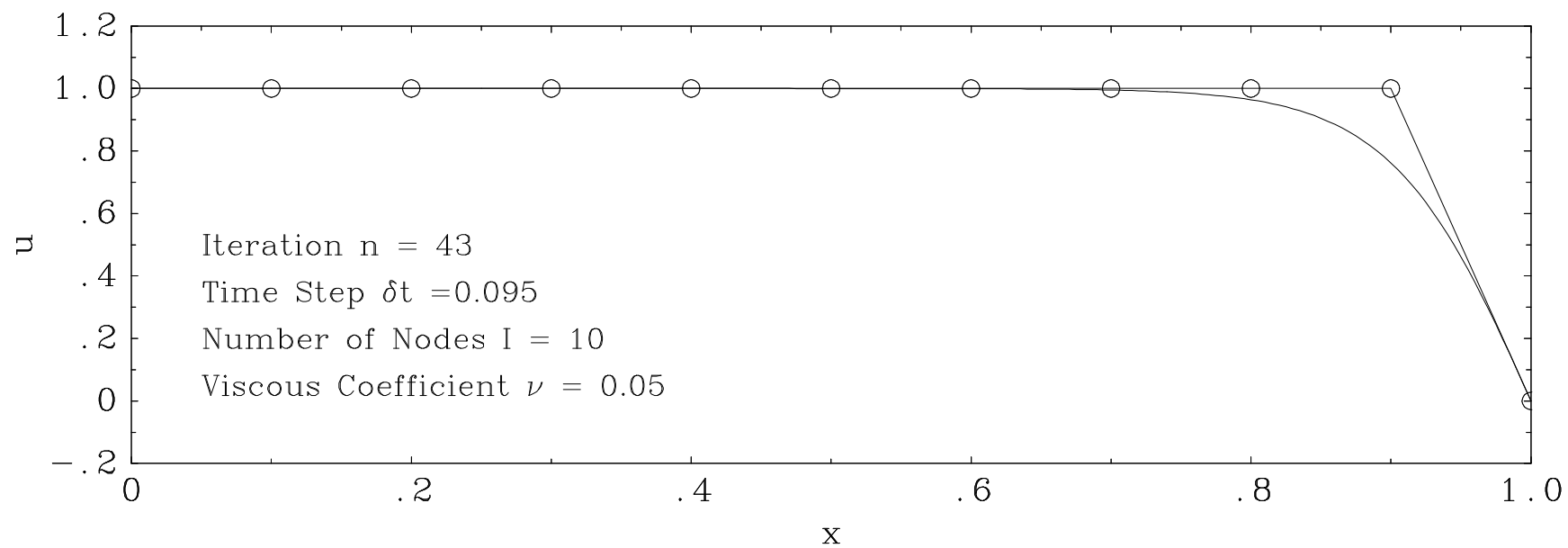
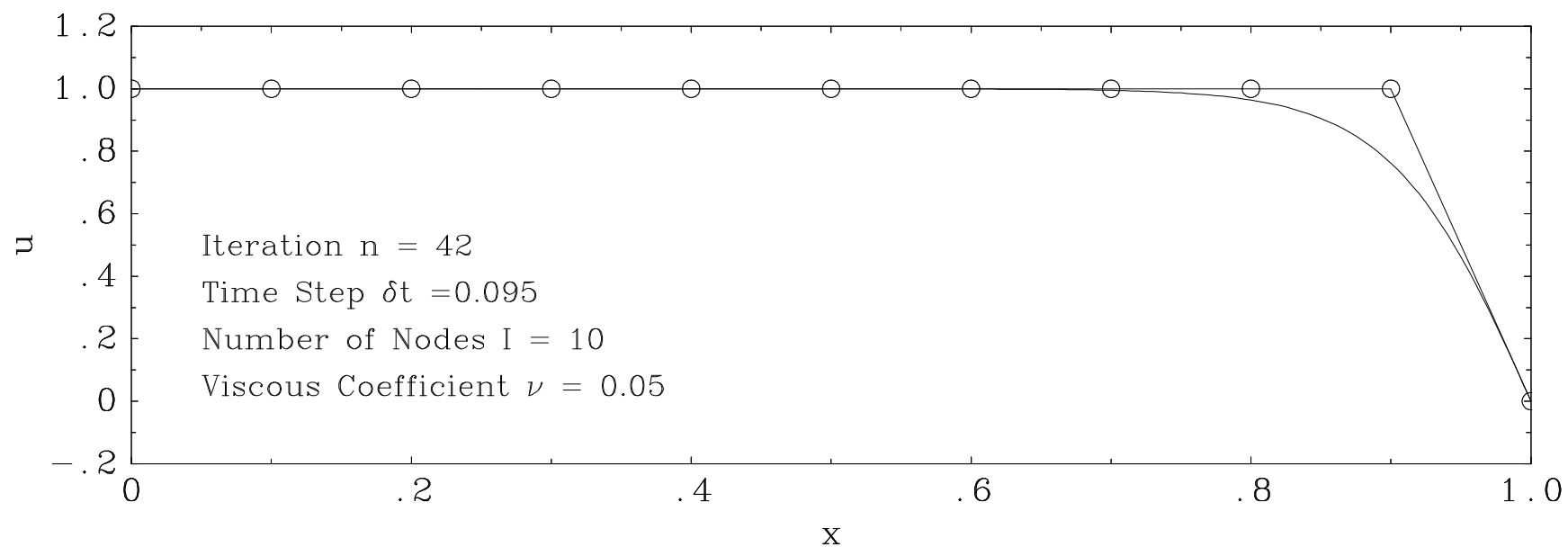
the scheme is stable. Unfortunately, the scheme is first order accurate in both space and time, and it introduces too much viscosity for problems involving hot gases.

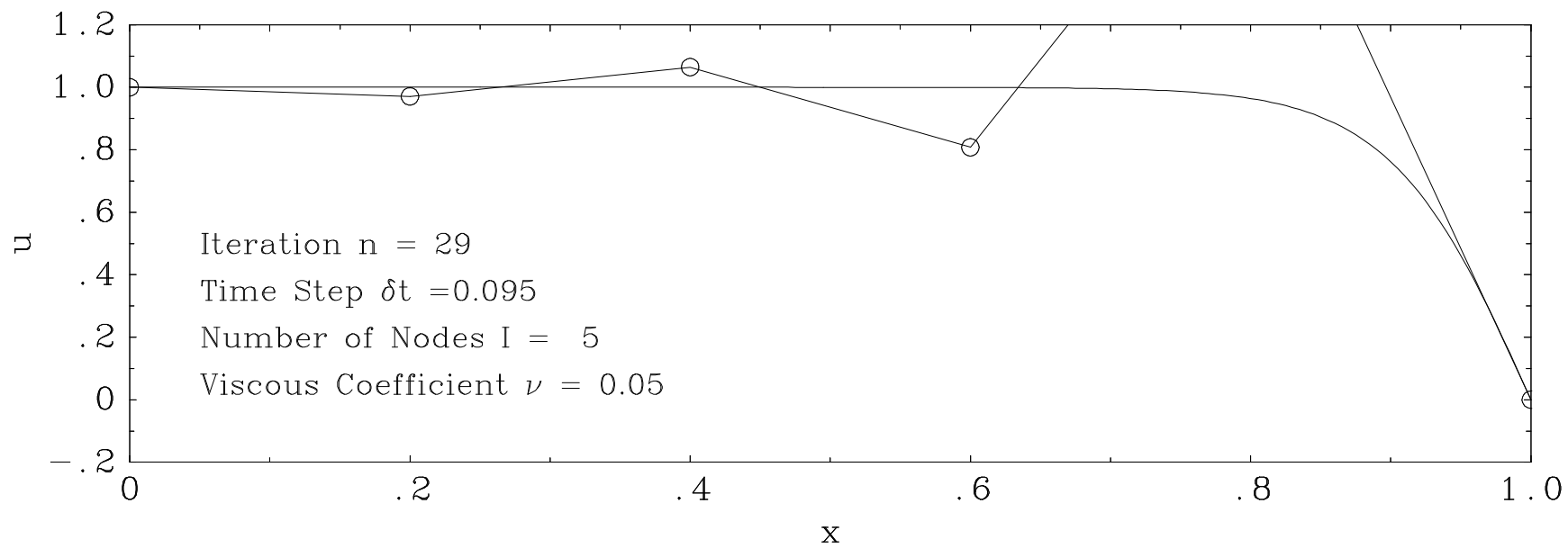
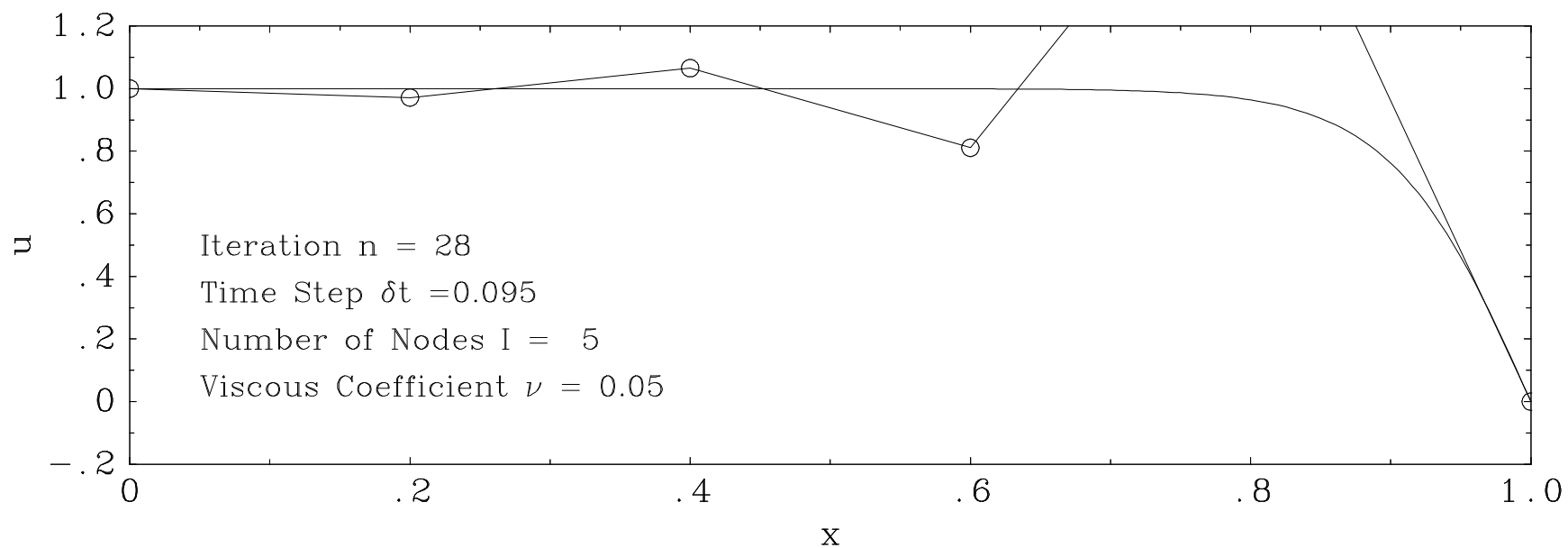
Lax's Equivalence Theorem

A general rule of CFD is that

$$\text{Consistency} + \text{Stability} \iff \text{Convergence}$$

If your scheme is consistent and stable, your solution will approach the exact solution as you use a finer and finer grid. Unfortunately, for all but the simplest of 1D problems, you are almost always limited by a grid of less than desirable resolution, especially for flows in which the flow variables make sharp transitions (*i.e.* steep gradients). Consider our model problem with less grid points:





Scalings and the Reynolds Number

Consider the N-S Equations for incompressible flow:

Mass Conservation

$$\nabla \cdot \mathbf{u} = 0$$

Momentum Conservation

$$\rho \frac{D\mathbf{u}}{Dt} + \nabla \tilde{p} = \mu \nabla^2 \mathbf{u}$$

What are the unknowns? u, v, w, \tilde{p}

ρ , the density, and μ , the dynamic viscosity, are constant. The equations can be non-dimensionalized with the velocity scaled by U , lengths scaled by L , and time scaled by L/U :

$$\mathbf{u}^* = \frac{\mathbf{u}}{U} \quad ; \quad \tilde{p}^* = \frac{\tilde{p}}{\rho U^2} \quad ; \quad t^* = \frac{U}{L} t \quad ; \quad \mathbf{x}^* = \frac{\mathbf{x}}{L} \quad ; \quad \nabla^* = L \nabla$$

The equations are rewritten

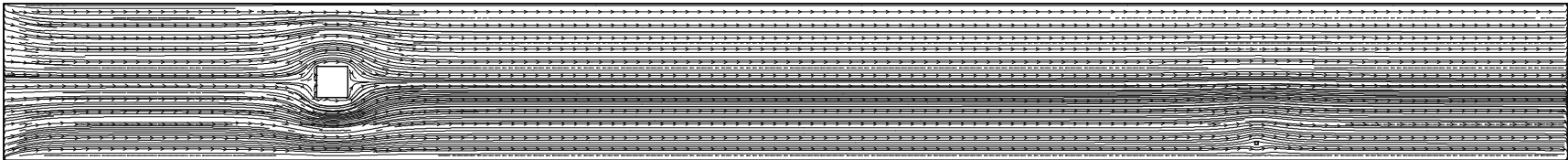
$$\begin{aligned} \nabla^* \cdot \mathbf{u}^* &= 0 \\ \frac{D\mathbf{u}^*}{Dt^*} + \nabla^* \tilde{p}^* &= \frac{\mu}{\rho UL} \nabla^{*2} \mathbf{u}^* \end{aligned}$$

The non-dimensional quantity $\rho UL/\mu$ is called the Reynolds number. For air at room temperature, $\mu = 1.8 \times 10^{-5} \text{ kg/(m s)}$, $\rho = 1.2 \text{ kg/m}^3$. For a typical room fire scenario, flow speeds are on the order of 10 m/s, length scales are on the order of 1-10 m. Thus, the Reynolds numbers are on the order of 0.5 million to 10 million.

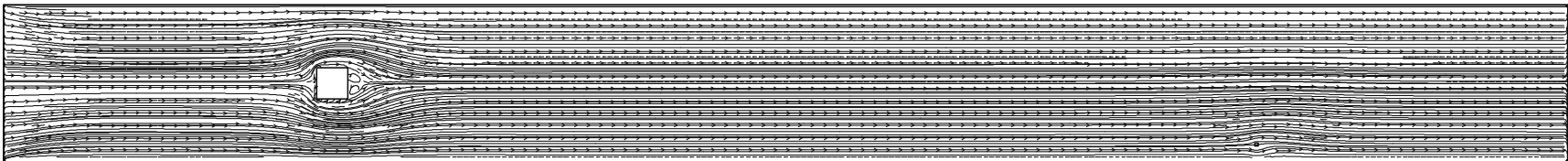
Reynolds Number Example

Consider the flow over an obstacle with a square cross section in an infinitely wide channel for Reynolds numbers of 1, 10, 100, and 1000.

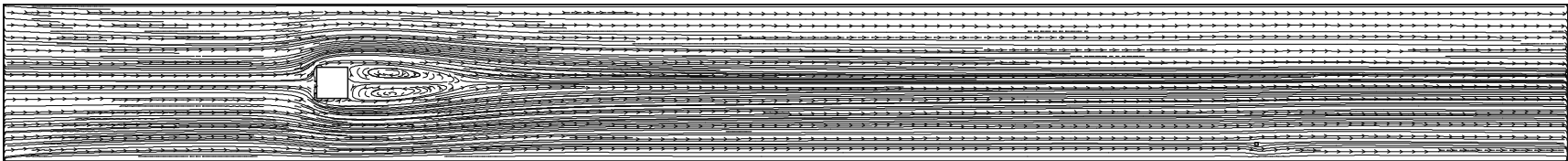
REYNOLDS NUMBER = 1



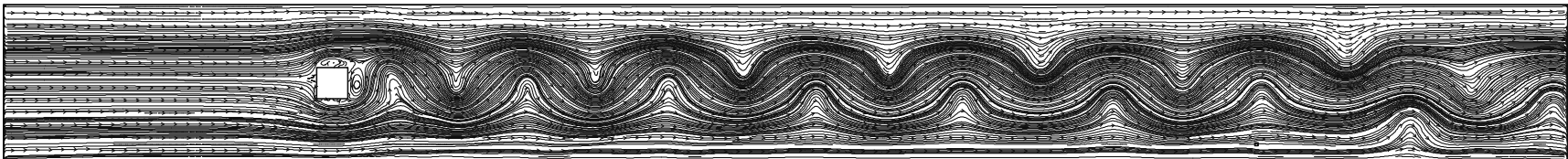
REYNOLDS NUMBER = 10



REYNOLDS NUMBER = 100



REYNOLDS NUMBER = 1000



What's the problem with high Reynolds numbers? Consider again Burgers Equation, and non-dimensionalize it

$$\frac{\partial u^*}{\partial t^*} + u^* \frac{\partial u^*}{\partial x^*} = \frac{1}{\text{Re}} \frac{\partial^2 u^*}{\partial x^{*2}}$$

where $u^*(x^*, t^*)$ is defined for $0 \leq x^* \leq 1$ with initial conditions

$$u^*(x^*, 0) = f(x^*)$$

and boundary conditions

$$u^*(0, t^*) = 1 \quad ; \quad u^*(1, t^*) = 0$$

Physically, this equation approximates the flow of a fluid between two flat, parallel plates, where x^* is the spatial coordinate normal to the plate, normalized by half the distance between the plates. The origin is the half-way point between the plates ($x^* = 0$), and one of the plates is at $x^* = 1$. Only half the flow is being considered, the other half is a mirror image. The velocity $u^* = 1$ represents the free-stream velocity. If the channel is 1 m wide, the free-stream velocity is $U = 1$ m/s, and the fluid is air, the Reynolds number (based on U and a characteristic length of half the channel width $L = 0.5$ m) is 33,333. The governing equation would be

$$\frac{\partial u^*}{\partial t^*} + u^* \frac{\partial u^*}{\partial x^*} = 3 \times 10^{-5} \frac{\partial^2 u^*}{\partial x^{*2}}$$

Recall the stability requirement for our simple central-difference numerical scheme

$$\delta t < \frac{2(3 \times 10^{-5})}{u^{*2}}$$

meaning that very small time steps will be needed to solve numerically, plus a lot of grid points will be needed to resolve the part of the flow field near the wall. For 2D and 3D problems with more complicated geometries and even higher Reynolds numbers, it's impossible even with the fastest computers and better numerical schemes to "resolve" this boundary layer. Worse yet, at these high Reynolds numbers, the boundary layer, and the flow in general, will not be laminar, but rather turbulent. For very simple flows at low Reynolds number, it is possible to do a Direct Numerical Simulation (DNS). For practical problems, some form of turbulence model will have to be used.

Time-Averaging and Turbulence Modeling

Decompose the flow quantities u , v , w , p , *etc.* into a time-averaged component and a fluctuating component

$$u(\mathbf{x}, t) = \bar{u}(\mathbf{x}, t) + u'(\mathbf{x}, t)$$

where

$$\bar{u}(\mathbf{x}, t) = \frac{1}{\Delta t} \int_{t-\Delta t/2}^{t+\Delta t/2} u(\mathbf{x}, t) dt$$

Δt is assumed large compared to the period of the fluctuations, but small compared to the characteristic time of the large scale motion. Note that

$$\overline{u'}(\mathbf{x}, t) = \frac{1}{\Delta t} \int_{t-\Delta t/2}^{t+\Delta t/2} u'(\mathbf{x}, t) dt = 0$$

but $\overline{u'u'} \neq 0$. The turbulent kinetic energy is often denoted

$$\frac{1}{2}(\overline{u'u'} + \overline{v'v'} + \overline{w'w'})$$

Reynolds Equations for Turbulent Flows

Apply time-averaging procedure to the incompressible N-S Equations:

$$\frac{1}{\Delta t} \int_{t-\Delta t/2}^{t+\Delta t/2} \left(\frac{\partial(\bar{u} + u')}{\partial x} + \frac{\partial(\bar{v} + v')}{\partial y} + \frac{\partial(\bar{w} + w')}{\partial z} \right) dt = 0$$

becomes

$$\frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{v}}{\partial y} + \frac{\partial \bar{w}}{\partial z} = 0$$

Thus, the mass conservation equation remains the same (because it is linear in u , v and w). However, the momentum equations are not linear, and after much manipulation the equations are rewritten

$$\begin{aligned} \rho \frac{D\bar{u}}{Dt} + \frac{\partial \bar{p}}{\partial x} &= \mu \left(\frac{\partial^2 \bar{u}}{\partial x^2} + \frac{\partial^2 \bar{u}}{\partial y^2} + \frac{\partial^2 \bar{u}}{\partial z^2} \right) - \rho \left(\frac{\partial(\overline{u'u'})}{\partial x} + \frac{\partial(\overline{u'v'})}{\partial y} + \frac{\partial(\overline{u'w'})}{\partial z} \right) \\ \rho \frac{D\bar{v}}{Dt} + \frac{\partial \bar{p}}{\partial y} &= \mu \left(\frac{\partial^2 \bar{v}}{\partial x^2} + \frac{\partial^2 \bar{v}}{\partial y^2} + \frac{\partial^2 \bar{v}}{\partial z^2} \right) - \rho \left(\frac{\partial(\overline{v'u'})}{\partial x} + \frac{\partial(\overline{v'v'})}{\partial y} + \frac{\partial(\overline{v'w'})}{\partial z} \right) \\ \rho \frac{D\bar{w}}{Dt} + \frac{\partial \bar{p}}{\partial z} &= \mu \left(\frac{\partial^2 \bar{w}}{\partial x^2} + \frac{\partial^2 \bar{w}}{\partial y^2} + \frac{\partial^2 \bar{w}}{\partial z^2} \right) - \rho \left(\frac{\partial(\overline{w'u'})}{\partial x} + \frac{\partial(\overline{w'v'})}{\partial y} + \frac{\partial(\overline{w'w'})}{\partial z} \right) \end{aligned}$$

Modeling the Reynolds Stresses

The Reynolds form of the N-S Equations look a lot like the original set derived above, but now there is the inclusion of another stress tensor, called the Reynolds stresses

$$\rho \frac{D\bar{\mathbf{u}}}{Dt} = -\nabla \bar{p} + \nabla \cdot (\bar{\boldsymbol{\tau}}_{lam} + \bar{\boldsymbol{\tau}}_{turb})$$

where the turbulent stress tensor is denoted

$$\bar{\boldsymbol{\tau}}_{turb} = -\rho \overline{u'_i u'_j} = \begin{pmatrix} -\rho \overline{u' u'} & -\rho \overline{u' v'} & -\rho \overline{u' w'} \\ -\rho \overline{v' u'} & -\rho \overline{v' v'} & -\rho \overline{v' w'} \\ -\rho \overline{w' u'} & -\rho \overline{w' v'} & -\rho \overline{w' w'} \end{pmatrix}$$

What is $-\rho \overline{u'_i u'_j}$? How shall these terms be modeled? The simplest approach is to say

$$-\rho \overline{u'_i u'_j} = \mu_t \frac{\partial \bar{u}_i}{\partial x_j}$$

where $\mu_t \gg \mu$ is a constant “eddy viscosity”. The u component of the momentum equation would then be

$$\rho \frac{D\bar{u}}{Dt} + \frac{\partial \bar{p}}{\partial x} = \mu \left(\frac{\partial^2 \bar{u}}{\partial x^2} + \frac{\partial^2 \bar{u}}{\partial y^2} + \frac{\partial^2 \bar{u}}{\partial z^2} \right) + \mu_t \left(\frac{\partial^2 \bar{u}}{\partial x^2} + \frac{\partial^2 \bar{u}}{\partial y^2} + \frac{\partial^2 \bar{u}}{\partial z^2} \right)$$

The “eddy viscosity” approach is regarded by many as overly simplistic, and a more common turbulence model (known as the $k - \varepsilon$ model) is

$$-\overline{u'_i u'_j} = \frac{\mu_t}{\rho} \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} k$$

where μ_t is a non-constant turbulent viscosity and k is the turbulent kinetic energy $\frac{1}{2}\overline{u'_i u'_i}$. By dimensional analysis

$$\frac{\mu_t}{\rho} \sim \frac{k^2}{\varepsilon} \quad \text{or} \quad \frac{\mu_t}{\rho} = c_1 \frac{k^2}{\varepsilon}$$

where ε is the dissipation rate of energy. There is a need now for two transport equations for k and ε

$$\begin{aligned} \frac{Dk}{Dt} &= \nabla \cdot \left(c_2 \frac{\mu_t}{\rho} \nabla k \right) + G - \varepsilon \\ \frac{D\varepsilon}{Dt} &= \nabla \cdot \left(c_3 \frac{\mu_t}{\rho} \nabla \varepsilon \right) + c_4 \frac{\varepsilon}{k} G - c_5 \frac{\varepsilon^2}{k} \\ G &= \frac{\mu_t}{\rho} \left[2 \left(\frac{\partial \bar{u}}{\partial x} \right)^2 + 2 \left(\frac{\partial \bar{v}}{\partial y} \right)^2 + 2 \left(\frac{\partial \bar{w}}{\partial z} \right)^2 \right. \\ &\quad \left. + \left(\frac{\partial \bar{u}}{\partial y} + \frac{\partial \bar{v}}{\partial x} \right)^2 + \left(\frac{\partial \bar{u}}{\partial z} + \frac{\partial \bar{w}}{\partial x} \right)^2 + \left(\frac{\partial \bar{v}}{\partial z} + \frac{\partial \bar{w}}{\partial y} \right)^2 \right] \end{aligned}$$

with the constants empirically derived

$$c_1 = 0.09 \quad ; \quad c_2 = 1.00 \quad ; \quad c_3 = 0.769 \quad ; \quad c_4 = 1.44 \quad ; \quad c_5 = 1.92$$

Large Eddy Simulation

Filter the flow quantities u, v, w, p , *etc.* as follows

$$\bar{u}(\mathbf{x}, t) = \int G(\mathbf{x}, \mathbf{x}') u(\mathbf{x}', t) d\mathbf{x}'$$

As before $\overline{u'u'} \neq 0$ and the momentum equation becomes

$$\rho \frac{D\bar{\mathbf{u}}}{Dt} = -\nabla \bar{p} + \nabla \cdot (\bar{\boldsymbol{\tau}}_{lam} + \bar{\boldsymbol{\tau}}_{turb})$$

where now

$$\bar{\tau}_{ij,turb} = -\rho(\overline{u_i u_j} - \bar{u}_i \bar{u}_j)$$

is the subgrid scale Reynolds stress. The simplest model of the subgrid scale Reynolds stress is

$$\bar{\boldsymbol{\tau}}_{turb} = \mu_{turb} \left(2 \text{def } \bar{\mathbf{u}} - \frac{2}{3} (\nabla \cdot \bar{\mathbf{u}}) \mathbf{I} \right)$$

where \mathbf{I} is the identity matrix and the deformation tensor is defined

$$\text{def } \bar{\mathbf{u}} \equiv \frac{1}{2} [\nabla \bar{\mathbf{u}} + (\nabla \bar{\mathbf{u}})^t] = \begin{pmatrix} \frac{\partial u}{\partial x} & \frac{1}{2} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) & \frac{1}{2} \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \\ \frac{1}{2} \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) & \frac{\partial v}{\partial y} & \frac{1}{2} \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \\ \frac{1}{2} \left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right) & \frac{1}{2} \left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right) & \frac{\partial w}{\partial z} \end{pmatrix}$$

The original Smagorinsky model for the viscous coefficient is

$$\mu_{turb} = \rho (C_s \Delta)^2 \left(2(\text{def } \bar{\mathbf{u}}) \cdot (\text{def } \bar{\mathbf{u}}) - \frac{2}{3}(\nabla \cdot \bar{\mathbf{u}})^2 \right)^{\frac{1}{2}}$$

with $C_s \approx 0.2$ and Δ roughly the size of the grid cell. Recall the Dissipation Function from the derivation of the energy equation

$$\begin{aligned} \Phi &\equiv \boldsymbol{\tau} \cdot \nabla \mathbf{u} \equiv \mu \left(2(\text{def } \mathbf{u}) \cdot (\text{def } \mathbf{u}) - \frac{2}{3}(\nabla \cdot \mathbf{u})^2 \right) \\ &= \mu \left[2 \left(\frac{\partial u}{\partial x} \right)^2 + 2 \left(\frac{\partial v}{\partial y} \right)^2 + 2 \left(\frac{\partial w}{\partial z} \right)^2 + \right. \\ &\quad \left. \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right)^2 + \left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right)^2 + \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right)^2 - \frac{2}{3} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right)^2 \right] \end{aligned}$$

Numerical Method for Low Mach Number Navier-Stokes Equations

Conservation of Mass

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0$$

Conservation of Species

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot \rho Y_i \mathbf{u} = \nabla \cdot \rho D_i \nabla Y_i + \dot{W}_i$$

Conservation of Momentum

$$\rho \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla \tilde{p} - \tilde{\rho} \mathbf{g} = \mathbf{f} + \nabla \cdot \boldsymbol{\tau}$$

Conservation of Energy

$$\frac{\partial}{\partial t}(\rho h) + \nabla \cdot \rho h \mathbf{u} = \frac{dp_0}{dt} + \dot{q}''' + \nabla \cdot k \nabla T + \nabla \cdot \sum_i \rho h_i D_i \nabla Y_i - \nabla \cdot \mathbf{q}_r$$

Equation of State

$$p_0(t) = \rho T \mathcal{R} \sum_i \frac{Y_i}{M_i}$$

Assuming that the constant-pressure specific heat of the i th species $c_{p,i}$ is assumed to be independent of temperature, the enthalpy can be written

$$h = \sum_i h_i Y_i = T \sum_i c_{p,i} Y_i$$

Also, assuming that the ratio of specific heats γ for each species is that of a diatomic molecule, the specific heat is a function only of the molecular weight

$$c_{p,i} = \left(\frac{\gamma}{\gamma - 1} \right) \frac{\mathcal{R}}{M_i}$$

The state equation can be simplified

$$p_0(t) = \frac{\gamma - 1}{\gamma} \rho h$$

Taking the total (or material) derivative of the state equation yields an expression for the divergence of the fluid

$$\nabla \cdot \mathbf{u} = \frac{\gamma - 1}{\gamma p_0} \left(\dot{q}''' + \nabla \cdot k \nabla T + \nabla \cdot \sum_i \rho h_i D_i \nabla Y_i - \nabla \cdot \mathbf{q}_r \right) - \frac{1}{\gamma p_0} \frac{dp_0}{dt}$$

Integrating the divergence over the entire domain Ω of volume V yields a consistency condition for the background pressure $p_0(t)$

$$\frac{dp_0}{dt} = \frac{\gamma - 1}{V} \left(\int_{\Omega} \dot{q}''' dV + \int_{\partial\Omega} k \nabla T \cdot d\mathbf{S} + \sum_i \int_{\partial\Omega} \rho h_i D_i \nabla Y_i \cdot d\mathbf{S} - \int_{\partial\Omega} \mathbf{q} \cdot d\mathbf{S} \right) - \frac{\gamma p_0}{V} \int_{\partial\Omega} \mathbf{u} \cdot d\mathbf{S}$$

Simplified Momentum Equation

Using the vector identity

$$(\mathbf{u} \cdot \nabla) \mathbf{u} = \frac{1}{2} \nabla |\mathbf{u}|^2 - \mathbf{u} \times \boldsymbol{\omega}$$

the momentum equation is written

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{1}{2} \nabla |\mathbf{u}|^2 - \mathbf{u} \times \boldsymbol{\omega} + \frac{1}{\rho} \nabla \tilde{p} - \frac{\tilde{\rho}}{\rho} \mathbf{g} = \frac{1}{\rho} (\mathbf{f} + \nabla \cdot \boldsymbol{\tau})$$

To simplify this equation further, a substitution is made

$$\nabla \mathcal{H} \approx \frac{1}{2} \nabla |\mathbf{u}|^2 + \frac{1}{\rho} \nabla \tilde{p}$$

Now the momentum equation becomes

$$\frac{\partial \mathbf{u}}{\partial t} - \mathbf{u} \times \boldsymbol{\omega} + \nabla \mathcal{H} - \frac{\tilde{\rho}}{\rho} \mathbf{g} = \frac{1}{\rho} (\mathbf{f} + \nabla \cdot \boldsymbol{\tau})$$

To obtain the pressure perturbation, we take the divergence of the momentum equation

$$\nabla \cdot \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{F} + \nabla \mathcal{H} \right) = 0$$

where all the convective and diffusive terms have been incorporated in the term \mathbf{F} . The resulting equation for the total pressure \mathcal{H} is an elliptic partial differential equation

$$\nabla^2 \mathcal{H} = -\frac{\partial(\nabla \cdot \mathbf{u})}{\partial t} - \nabla \cdot \mathbf{F}$$

The linear algebraic system arising from the discretization of this equation has constant coefficients and can be solved to machine accuracy by a fast, direct (*i.e.* non-iterative) method that utilizes fast Fourier transforms. No-flux boundary conditions are specified by asserting that

$$\frac{\partial \mathcal{H}}{\partial n} = -F_n$$

at external boundaries and

$$F_n = -\frac{\partial \mathcal{H}^{old}}{\partial n} + \frac{\beta u_n}{\delta t}$$

at internal boundaries, assuring that the normal component of velocity u_n will be driven closer to zero according to

$$\frac{\partial u_n}{\partial t} \approx -\beta u_n$$

LES vs. DNS

The components of the viscous stress tensor are given by

$$\boldsymbol{\tau} = \mu \left(2 \operatorname{def} \mathbf{u} - \frac{2}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right)$$

The viscous terms can be handled either by assuming a temperature-dependent dynamic viscosity

$$\mu = \mu_{\infty} \left(\frac{T}{T_{\infty}} \right)^{0.75}$$

or the sub-grid scale stresses can be modeled following Smagorinsky where the viscosity is given

$$\mu = \rho (C_s \Delta)^2 \left(2(\operatorname{def} \mathbf{u}) \cdot (\operatorname{def} \mathbf{u}) - \frac{2}{3} (\nabla \cdot \mathbf{u})^2 \right)^{\frac{1}{2}}$$

where C_s is an empirical constant, Δ is a length on the order of the size of a grid cell, and the deformation term is related to the Dissipation Function

$$\begin{aligned}
\Phi &\equiv \boldsymbol{\tau} \cdot \nabla \mathbf{u} \equiv \mu \left(2(\mathbf{def} \, \mathbf{u}) \cdot (\mathbf{def} \, \mathbf{u}) - \frac{2}{3}(\nabla \cdot \mathbf{u})^2 \right) \\
&= \mu \left[2 \left(\frac{\partial u}{\partial x} \right)^2 + 2 \left(\frac{\partial v}{\partial y} \right)^2 + 2 \left(\frac{\partial w}{\partial z} \right)^2 + \right. \\
&\quad \left. \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right)^2 + \left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right)^2 + \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right)^2 - \frac{2}{3} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right)^2 \right]
\end{aligned}$$

Time-Stepping

A simple way to iterate a differential equation for a function of time $\phi(t)$

$$\frac{d\phi}{dt} = f(\phi, t)$$

with initial condition $\phi(0) = \phi^0$.

Predictor step:

$$\phi^* = \phi^n + \delta t f(\phi^n, t^n) \quad t^n = n \delta t$$

Corrector step:

$$\phi^{n+1} = \phi^n + \frac{\delta t}{2} [f(\phi^n, t^n) + f(\phi^*, t^n + \delta t)]$$

The corrector step can be rewritten:

$$\phi^{n+1} = \frac{1}{2} [\phi^n + \phi^* + \delta t f(\phi^*, t^n + \delta t)]$$

Solution Procedure

1. The thermodynamic quantities ρ , Y_i , and p_0 are estimated at the next time step with an explicit Euler step. For example, the density is estimated

$$\rho^{(n+1)_e} = \rho^n - \delta t \nabla \cdot \rho^n \mathbf{u}^n$$

The divergence $(\nabla \cdot \mathbf{u})^{(n+1)_e}$ is formed from these estimated thermodynamic quantities.

2. A Poisson equation for the pressure is solved with a direct solver

$$\nabla^2 \mathcal{H}^n = -\frac{(\nabla \cdot \mathbf{u})^{(n+1)_e} - (\nabla \cdot \mathbf{u})^n}{\delta t} - \nabla \cdot \mathbf{F}^n$$

Then the velocity is estimated at the next time step

$$\mathbf{u}^{(n+1)_e} = \mathbf{u}^n - \delta t (\mathbf{F}^n + \nabla \mathcal{H}^n)$$

3. The thermodynamic quantities ρ , Y_i , and p_0 are corrected at the next time step. For example, the density is corrected

$$\rho^{n+1} = \frac{1}{2} \left(\rho^n + \rho^{(n+1)_e} - \delta t \nabla \cdot \rho^{(n+1)_e} \mathbf{u}^{(n+1)_e} \right)$$

The divergence $(\nabla \cdot \mathbf{u})^{(n+1)}$ is derived from the corrected thermodynamic quantities.

4. The pressure is recomputed using estimated quantities

$$\nabla^2 \mathcal{H}^{(n+1)_e} = -\frac{2(\nabla \cdot \mathbf{u})^{n+1} - (\nabla \cdot \mathbf{u})^{(n+1)_e} - (\nabla \cdot \mathbf{u})^n}{\delta t} - \nabla \cdot \mathbf{F}^{(n+1)_e}$$

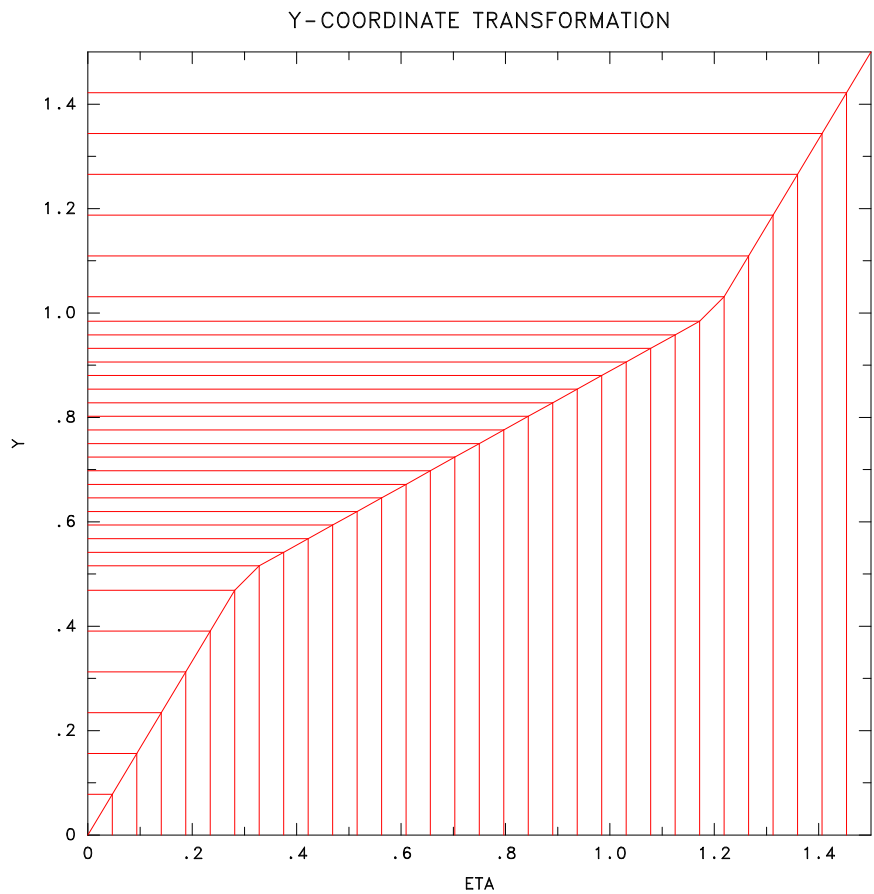
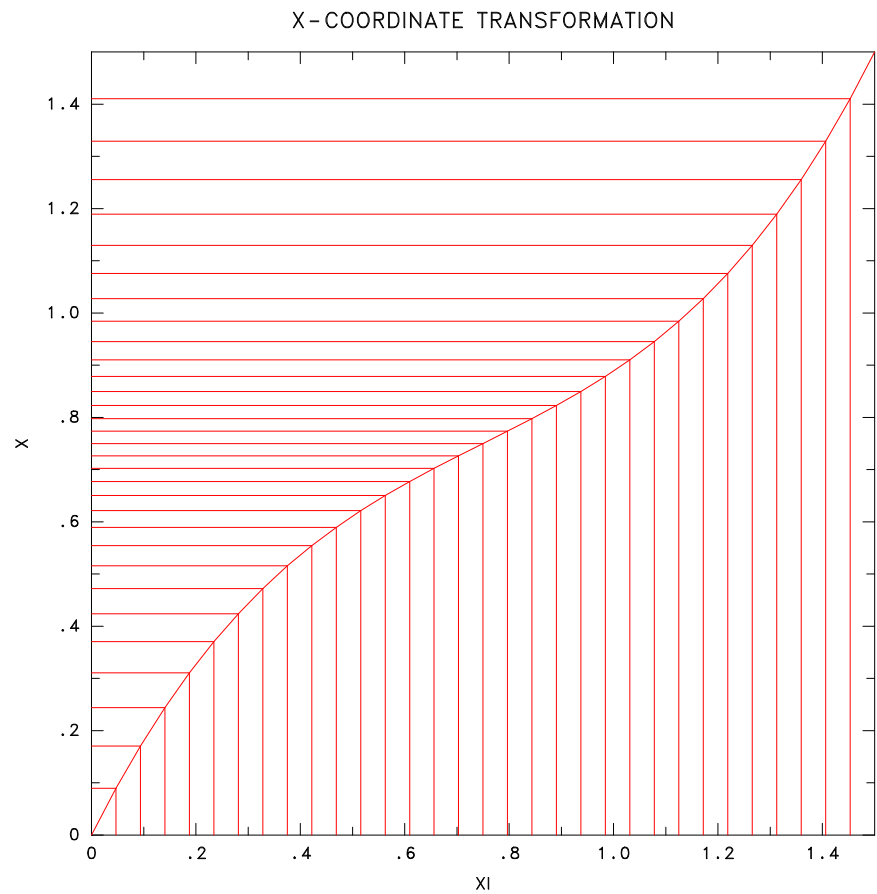
The velocity is then corrected

$$\mathbf{u}^{n+1} = \frac{1}{2} \left[\mathbf{u}^n + \mathbf{u}^{(n+1)_e} - \delta t \left(\mathbf{F}^{(n+1)_e} + \nabla \mathcal{H}^{(n+1)_e} \right) \right]$$

Coordinate Transformations

The grid dimensions δx , δy and δz can vary as functions of their respective spatial coordinate, *i.e.*

$$\delta x_i = \frac{df_x}{d\xi}(\xi_i) \delta\xi \quad ; \quad \delta y_j = \frac{df_y}{d\eta}(\eta_j) \delta\eta \quad ; \quad \delta z_k = \frac{df_z}{d\zeta}(\zeta_k) \delta\zeta$$

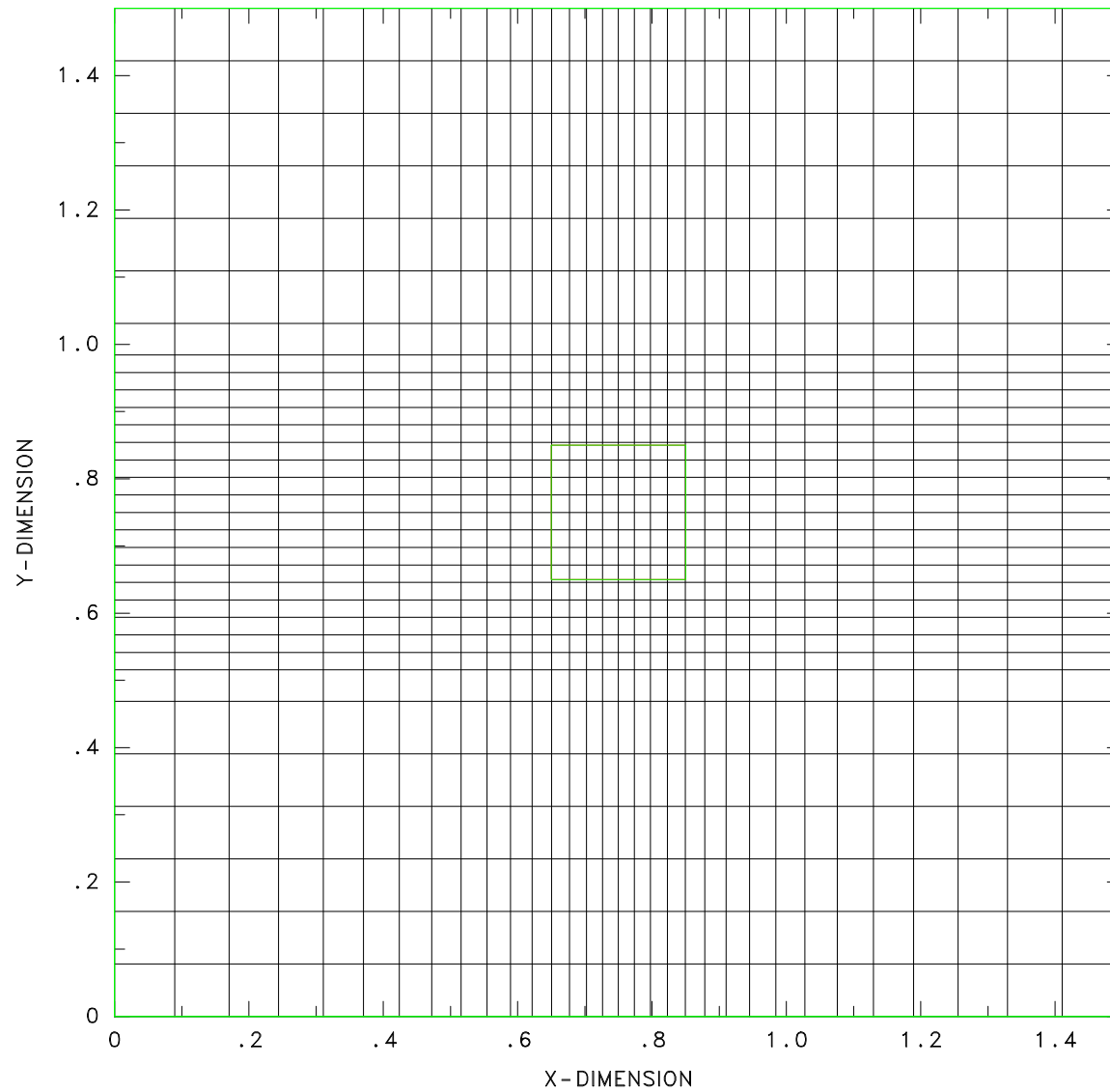


Polynomial Stretch

```
&TRAN IDERIV=0,CC=0.75,PC=0.75 /
&TRAN IDERIV=1,CC=0.75,PC=0.50 /
```

Piecewise Linear Stretch

```
&TRAN CC=0.30,PC=0.50 /
&TRAN CC=1.20,PC=1.00 /
```



Spatial Differences

The density at the center of the ijk th cell is updated in time with the following predictor-corrector scheme. In the predictor step, the density at the $(n+1)$ st time level is estimated based on information at the n th level

$$\frac{\rho_{ijk}^{(n+1)_e} - \rho_{ijk}^n}{\delta t} + (\mathbf{u} \cdot \nabla \rho)_{ijk}^n = -\rho_{ijk}^n (\nabla \cdot \mathbf{u})_{ijk}^n$$

Following the prediction of the velocity and background pressure at the $(n+1)$ st time level, the density is corrected

$$\frac{\rho_{ijk}^{(n+1)} - \frac{1}{2} \left(\rho_{ijk}^n + \rho_{ijk}^{(n+1)_e} \right)}{\frac{1}{2} \delta t} + (\mathbf{u} \cdot \nabla \rho)_{ijk}^{(n+1)_e} = -\rho_{ijk}^{(n+1)_e} (\nabla \cdot \mathbf{u})_{ijk}^{(n+1)_e}$$

The convective terms are written as upwind-biased differences in the predictor step and downwind-biased differences in the corrector step. In the expressions to follow, the symbol \pm means $+$ in the predictor step and $-$ in the corrector step. The opposite is true for \mp .

$$\begin{aligned} (\mathbf{u} \cdot \nabla \rho)_{ijk} = & \frac{1 \mp \epsilon_u}{2} u_{ijk} \frac{\rho_{i+1,jk} - \rho_{ijk}}{\delta x} + \frac{1 \pm \epsilon_u}{2} u_{i-1,jk} \frac{\rho_{ijk} - \rho_{i-1,jk}}{\delta x} + \\ & \frac{1 \mp \epsilon_v}{2} v_{ijk} \frac{\rho_{i,j+1,k} - \rho_{ijk}}{\delta y} + \frac{1 \pm \epsilon_v}{2} v_{i,j-1,k} \frac{\rho_{ijk} - \rho_{i,j-1,k}}{\delta y} + \\ & \frac{1 \mp \epsilon_w}{2} w_{ijk} \frac{\rho_{ij,k+1} - \rho_{ijk}}{\delta z} + \frac{1 \pm \epsilon_w}{2} w_{ij,k-1} \frac{\rho_{ijk} - \rho_{ij,k-1}}{\delta z} \end{aligned}$$

Note that without the inclusion of the ε 's, these are simple central difference approximations. The ε 's are local CFL numbers, $\varepsilon_u = u\delta t/\delta x$, $\varepsilon_v = v\delta t/\delta y$, and $\varepsilon_w = w\delta t/\delta z$, where the velocity components are those that immediately follow. Their role is to bias the differencing upwind. Where the local CFL number is near unity, the difference becomes nearly fully upwind. Where the local CFL number is much less than unity, the differencing is more centralized.

The divergence in both the predictor and corrector step is discretized

$$(\nabla \cdot \mathbf{u})_{ijk} = \frac{\gamma - 1}{\gamma p_0} \left(\dot{q}_{ijk}''' + (\nabla \cdot k \nabla T)_{ijk} + \sum_l (\nabla \cdot T c_{p,l} \rho D \nabla Y_l)_{ijk} - \frac{1}{\gamma - 1} \left(\frac{dp_0}{dt} \right) \right)$$

The thermal and material diffusion terms are pure central differences, with no upwind or downwind bias, thus they are differenced the same way in both the predictor and corrector steps

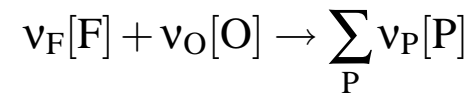
$$\begin{aligned} (\nabla \cdot k \nabla T)_{ijk} = & \frac{1}{\delta x} \left[k_{i+\frac{1}{2},jk} \frac{T_{i+1,jk} - T_{ijk}}{\delta x} - k_{i-\frac{1}{2},jk} \frac{T_{ijk} - T_{i-1,jk}}{\delta x} \right] + \\ & \frac{1}{\delta y} \left[k_{i,j+\frac{1}{2},k} \frac{T_{i,j+1,k} - T_{ijk}}{\delta y} - k_{i,j-\frac{1}{2},k} \frac{T_{ijk} - T_{i,j-1,k}}{\delta y} \right] + \\ & \frac{1}{\delta z} \left[k_{ij,k+\frac{1}{2}} \frac{T_{ij,k+1} - T_{ijk}}{\delta z} - k_{ij,k-\frac{1}{2}} \frac{T_{ijk} - T_{ij,k-1}}{\delta z} \right] \end{aligned}$$

The temperature is extracted from the density via the equation of state

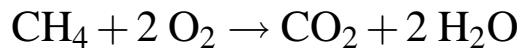
$$T_{ijk} = \frac{p_0}{\rho_{ijk} \mathcal{R} \sum_{l=0}^N (Y_{l,ijk} / M_l)}$$

Combustion

Start with the most general form of the combustion reaction



The numbers ν_i are the stoichiometric coefficients for the overall reaction of fuel “F” and oxygen “O” to produce products “P”. For example, ideal methane combustion is



Assuming mass consumption rates of fuel and oxygen are related

$$\frac{\dot{W}_F'''}{\nu_F M_F} = \frac{\dot{W}_O'''}{\nu_O M_O}$$

the mixture fraction Z is defined as:

$$Z = \frac{s Y_F - (Y_O - Y_O^\infty)}{s Y_F^\infty + Y_O^\infty} \quad ; \quad s = \frac{\nu_O M_O}{\nu_F M_F}$$

$Z = 1$ in the fuel stream, $Z = 0$ pure air, with $Y_O = Y_O^\infty \approx 0.23$. Note for methane

$$s = \frac{(2)(32)}{(1)(16)} = 4$$

The mixture fraction satisfies the conservation law

$$\begin{aligned}
 & \frac{s}{sY_F^\infty + Y_O^\infty} \left[\rho \frac{DY_F}{Dt} = \nabla \cdot \rho D \nabla Y_F + \dot{W}_F''' \right] \\
 + & \frac{-1}{sY_F^\infty + Y_O^\infty} \left[\rho \frac{D(Y_O - Y_O^\infty)}{Dt} = \nabla \cdot \rho D \nabla (Y_O - Y_O^\infty) + \dot{W}_O''' \right]
 \end{aligned}$$

$$\rho \frac{DZ}{Dt} = \nabla \cdot \rho D \nabla Z$$

obtained from a linear combination of the fuel and oxygen conservation equations.

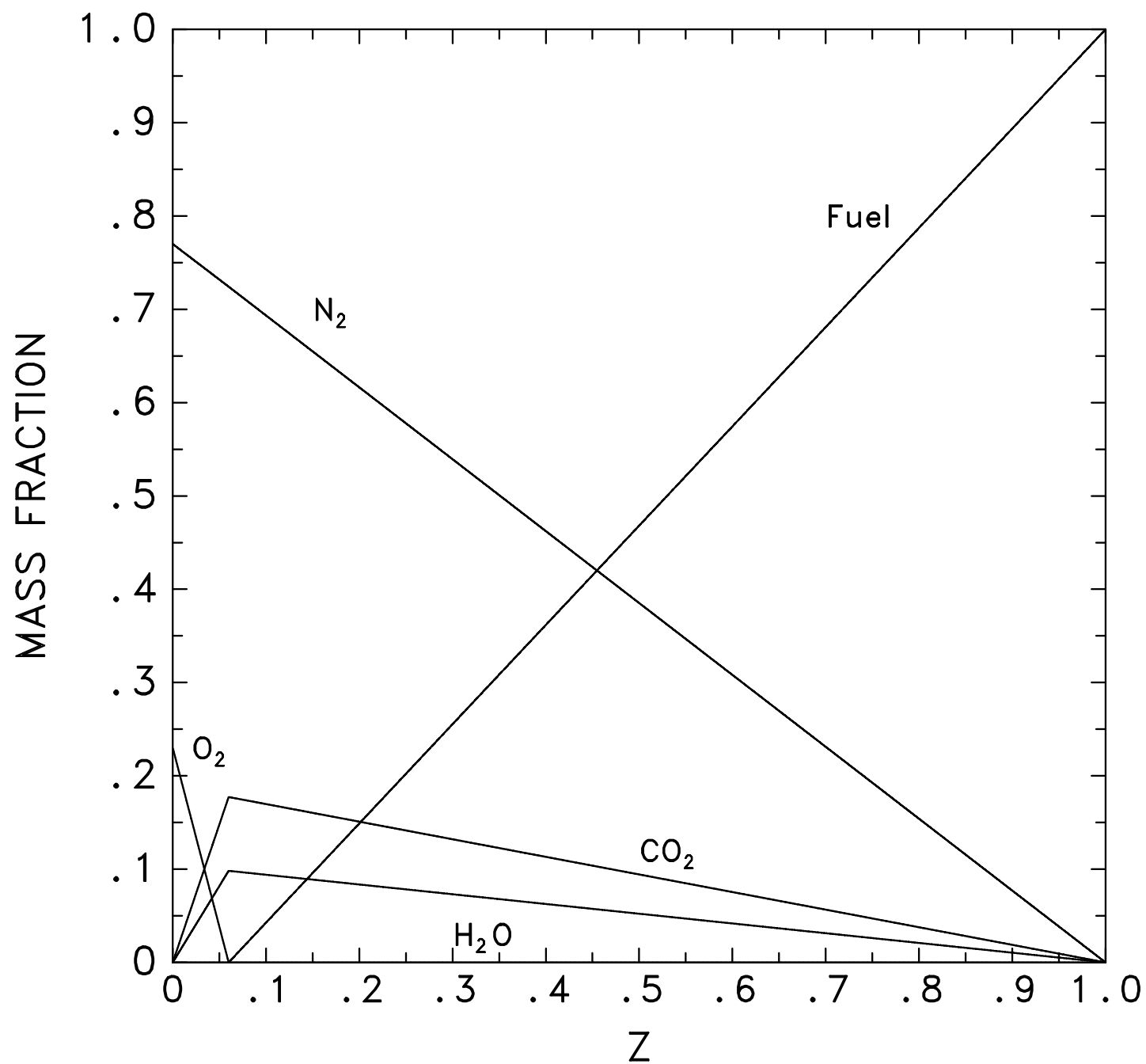
The assumption that fuel and oxygen vanish at the infinitely thin flame sheet

$$Z(\mathbf{x}, t) = Z_F \quad ; \quad Z_F = \frac{Y_O^\infty}{sY_F^\infty + Y_O^\infty}$$

yields the simplest state relation for oxygen as a function of Z

$$Y_O(Z) = \begin{cases} Y_O^\infty(1 - Z/Z_F) & Z < Z_F \\ 0 & Z > Z_F \end{cases}$$

This expression is known as the “state relation” for oxygen. It ties oxygen to the mixture fraction.



What is the heat release rate per unit volume \dot{q}''' ?

$$\dot{q}''' = \Delta H_O \dot{W}_O'''$$

Here, ΔH_O is the heat release rate per unit mass of oxygen consumed (about 13,100 kJ/kg). The oxygen mass conservation equation

$$\rho \frac{DY_O}{Dt} = \nabla \cdot \rho D \nabla Y_O + \dot{W}_O'''$$

can be transformed into an expression for the local heat release rate using the conservation equation for the mixture fraction and the state relation for oxygen $Y_O(Z)$.

$$\rho \frac{DY_O}{Dt} = \rho \frac{dY_O}{dZ} \frac{DZ}{Dt} = \frac{dY_O}{dZ} \nabla \cdot \rho D \nabla Z \quad ; \quad \rho D \nabla Y_O = \rho D \frac{dY_O}{dZ} \nabla Z$$

Yielding:

$$-\dot{W}_O''' = \nabla \cdot \left(\rho D \frac{dY_O}{dZ} \nabla Z \right) - \frac{dY_O}{dZ} \nabla \cdot \rho D \nabla Z$$

This expression for the local oxygen consumption rate is not particularly convenient to apply numerically because of the discontinuity of the derivative of $Y_O(Z)$ at $Z = Z_F$. A better expression is the oxygen consumption rate *per unit area* of the flame sheet

$$-\dot{W}_O'' = \left. \frac{dY_O}{dZ} \right|_{Z=Z_F} \rho D \nabla Z \cdot \mathbf{n}$$

In the numerical algorithm, the local heat release rate is computed by first locating the flame sheet, then computing the local heat release rate per unit area, and finally distributing this energy to the grid cells cut by the flame sheet.

The total HRR is given by

$$\dot{Q} = \Delta H_O \int_F -\dot{m}''_O dA = \Delta H_O \int_F \frac{dY_O}{dZ} \rho D \nabla Z \cdot d\mathbf{S}$$

$$\Delta H_O \approx 13,100 \text{ kJ/kg O}_2 \quad ; \quad \frac{dY_O}{dZ} = -\frac{0.23}{Z_F}$$

Coarse Grid Considerations

Return to the transport equation for the mixture fraction in conservative form:

$$\frac{\partial(\rho Z)}{\partial t} + \nabla \cdot \rho \mathbf{u} Z = \nabla \cdot \rho D \nabla Z$$

Integrating over the flaming volume

$$\int_{B+F} \rho \mathbf{u} Z \cdot d\mathbf{S} \approx \int_{B+F} \rho D \nabla Z \cdot d\mathbf{S}$$

Rearrange terms

$$(1 - Z_F) \dot{m} = - \int_F \rho D \nabla Z \cdot d\mathbf{S} \quad ; \quad (1 - Z_F) \frac{dY_O}{dZ} \Delta H_O = \Delta H$$

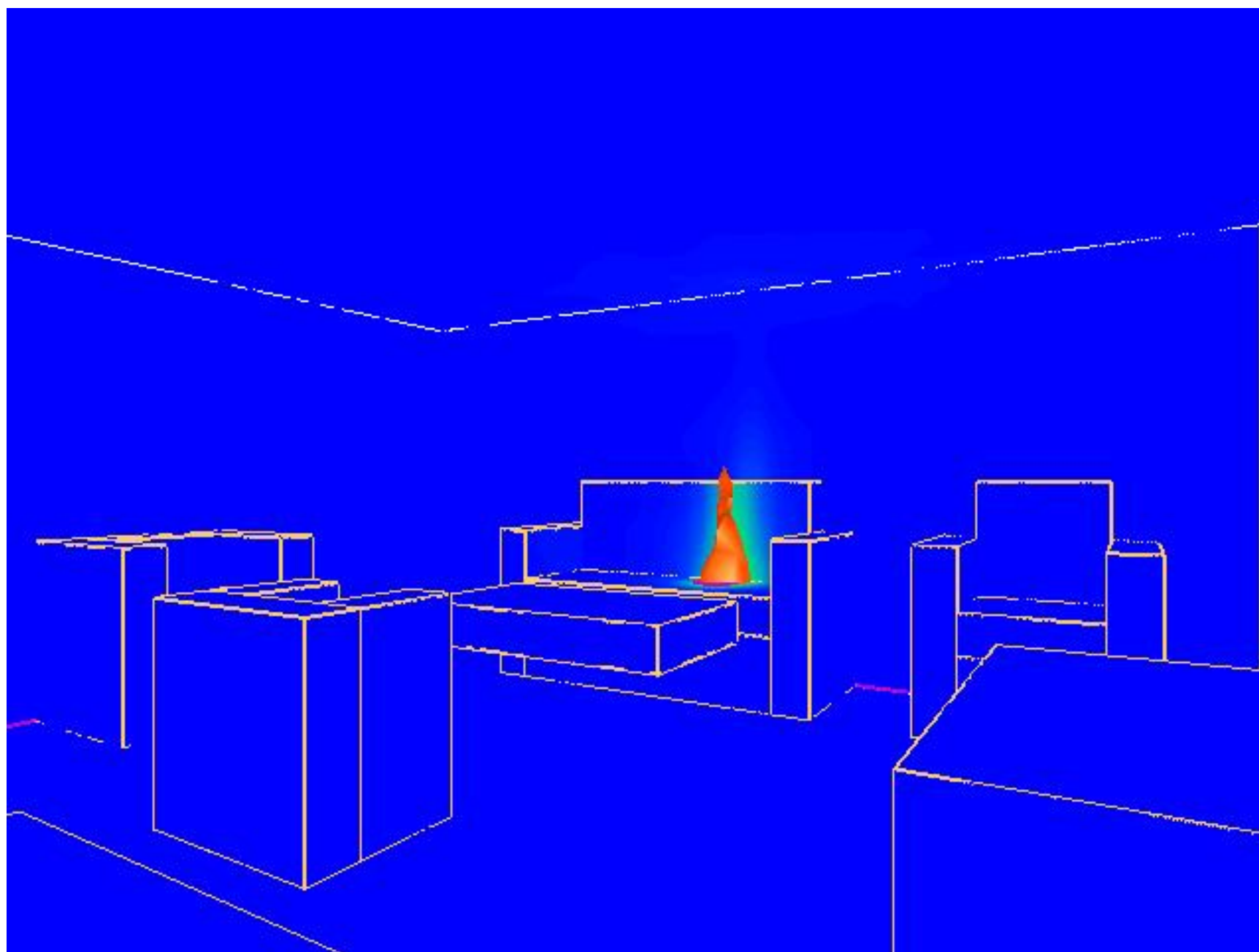
Suppose we choose a different value of Z_F . We can still recover the desired HRR by integrating over a “different” flame, $Z_{F,e}$, if

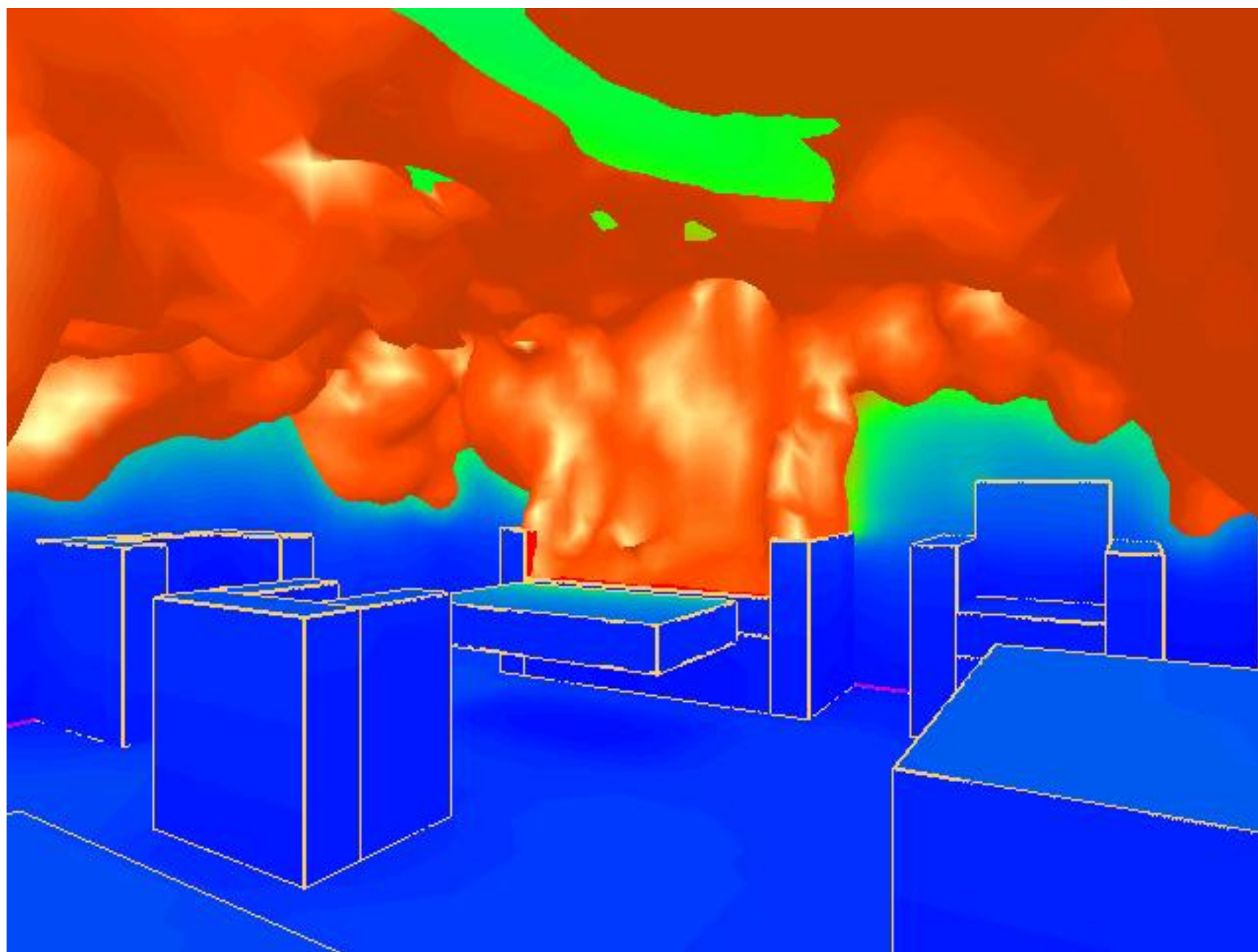
$$\left(\frac{dY_O}{dZ} \right)_e = \frac{\Delta H / \Delta H_O}{(1 - Z_{F,e})}$$

What should we choose for $Z_{F,e}$? Empirically, it has been found that a good choice is

$$\frac{Z_{F,e}}{Z_F} = \min \left(1, C \frac{D^*}{\delta x} \right)$$

For “well-resolved” grids $Z_{F,e} = Z_F$, but for less-resolved grids, $Z_{F,e} < Z_F$. The value of $Z_{F,e}$ will approach Z_F as the fire grows.





Strengths of Mixture Fraction Approach

- Only one additional scalar convective/diffusion equation to solve
- Infinite rate combustion consistent with LES length and time scales
- Many product species can be expressed as functions of mixture fraction

Weaknesses of Mixture Fraction Approach

- Diffusion coefficient the same for all gas species
- Infinite rate kinetics, no support for detailed flame structure
- Fuel and oxygen always react eventually, regardless of temperature

Dimensional Analysis

Characteristic length scale for fire plume correlations:

$$D^* = \left(\frac{\dot{Q}}{\rho_{\infty} c_p T_{\infty} \sqrt{g}} \right)^{2/5} ; \quad Q^* = \frac{\dot{Q}}{\rho_{\infty} c_p T_{\infty} \sqrt{g} D^{5/2}} ; \quad Q^* = \left(\frac{D^*}{D} \right)^{5/2}$$

Where does this characteristic length come from? Consider the Energy Conservation equation

$$\rho c_p \frac{DT}{Dt} = \dot{q}''' + \nabla \cdot k \nabla T + \dots$$

Non-dimensionalize according to

$$\mathbf{x}^* = \mathbf{x}/D^* ; \quad \mathbf{u}^* = \mathbf{u}/\sqrt{g D^*} ; \quad t^* = t/\sqrt{D^*/g} ; \quad \rho^* = \rho/\rho_{\infty} ; \quad T^* = T/T_{\infty}$$

The Energy equation is now written in non-dimensional form

$$\rho^* \frac{DT^*}{Dt^*} = \dot{q}'''^* + \nabla \cdot k^* \nabla T^* + \dots$$

where

$$\dot{q}'''^* = \frac{\sqrt{D^*}}{\rho_{\infty} c_p T_{\infty} \sqrt{g}} \dot{q}'''$$

Integrating the local HRR over the entire domain

$$\int \dot{q}'''^* dV^* = \frac{\int \dot{q}''' dV}{\rho_{\infty} c_p T_{\infty} \sqrt{g} D^{*5/2}} = 1$$

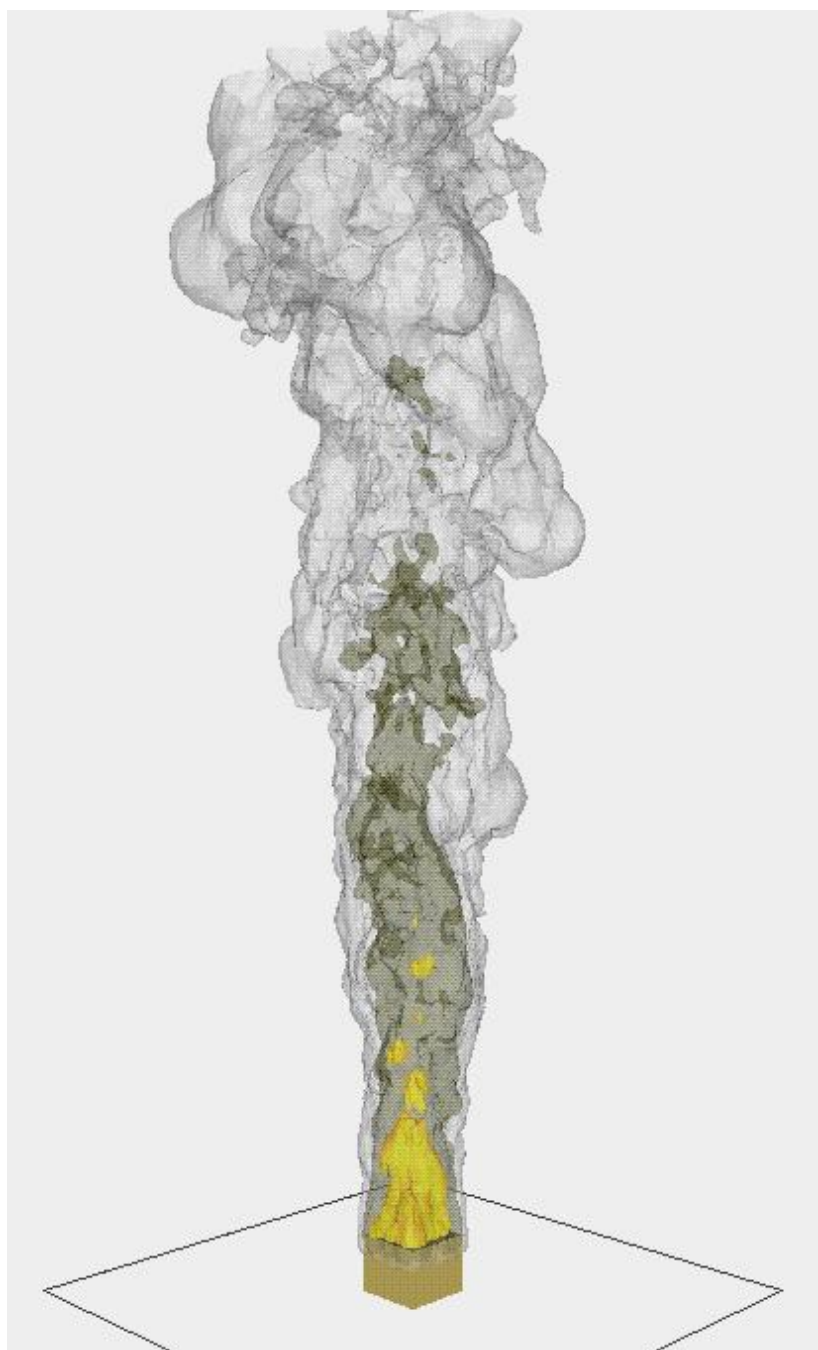
What does this mean? Developers of engineering correlations for plumes and other fire-driven flows built into the formulae nondimensional quantities allowing one to scale from small to large fires. Since the correlations are derived from the equations of motion being solved numerically, they retain this character. A single plume calculation can be scaled for fires of about $D^* = 10$ cm to fires of 10 m and beyond. As long as a sufficient number of grid cells span D^* , the major plume structures will be captured in the calculation. The quality of the calculation is determined by

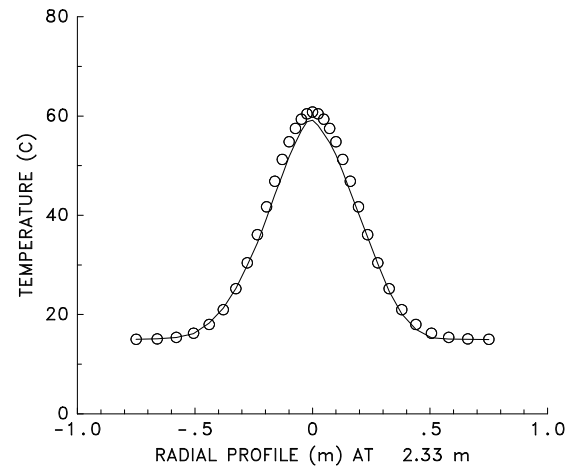
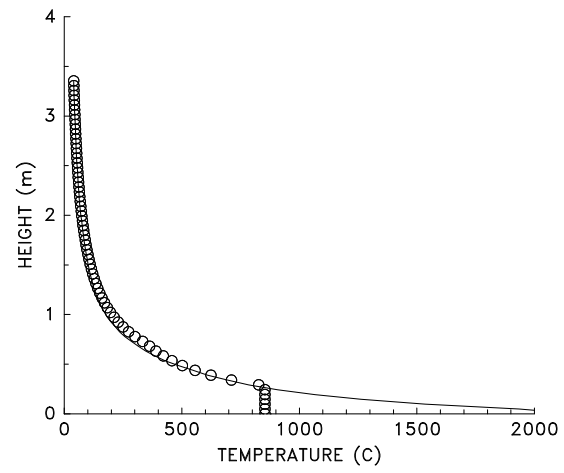
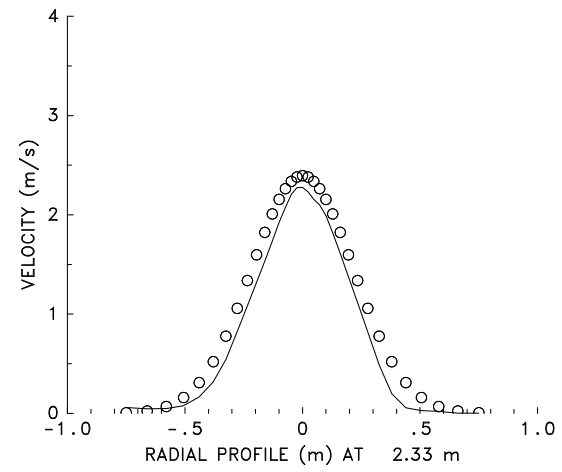
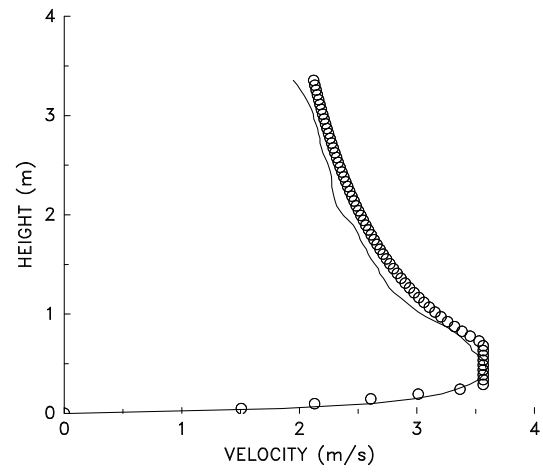
$$D^*/\delta x$$

When $D^*/\delta x$ is relatively small, the surface $Z = Z_F$ shrinks closer to the burner surface because of numerical diffusion of the fuel stream. It has been found empirically that a good estimate of flame height can be found for crude grids if a different value of Z is used to define the combustion region

$$\frac{Z_{F,e}}{Z_F} = \min \left(1, C \frac{D^*}{\delta x} \right)$$

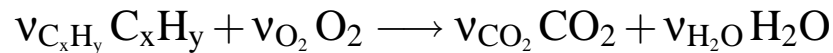
As $D^*/\delta x$ increases, $Z_{F,e} \rightarrow Z_F$.





Finite-rate Combustion

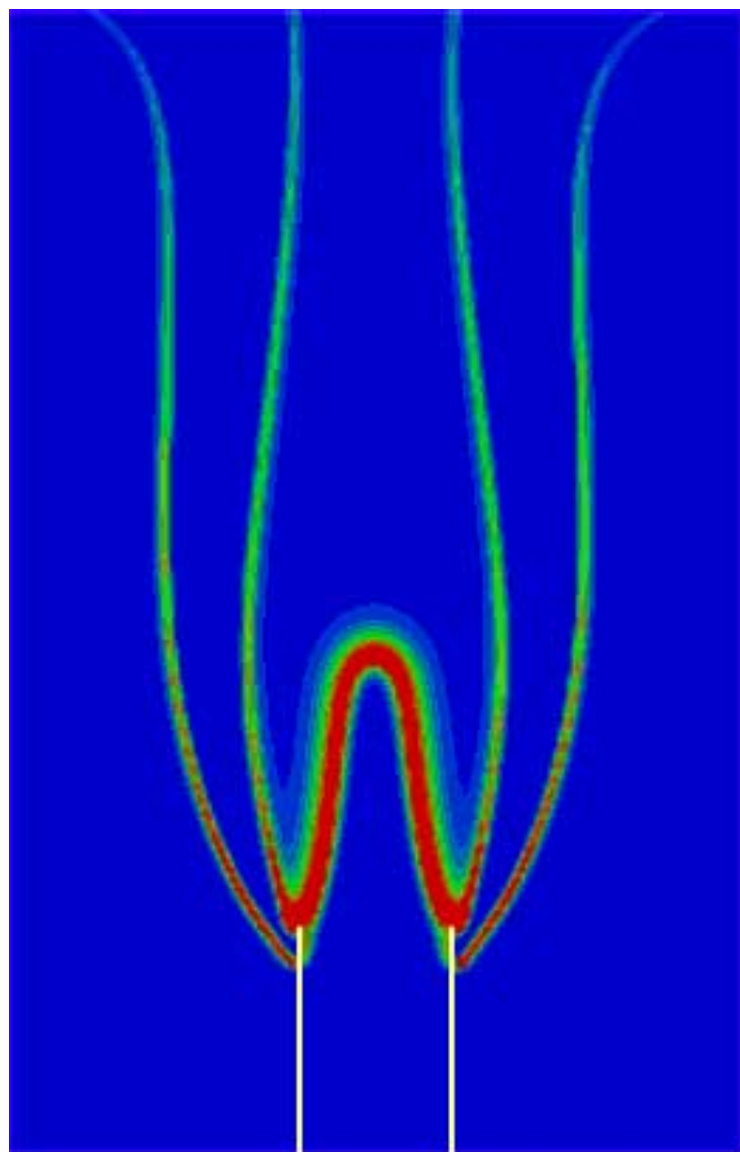
In a DNS calculation, the diffusion of fuel and oxygen can be modeled directly, thus it is possible to implement a single or multiple step chemical reaction. Consider the (single) reaction of oxygen and a hydrocarbon fuel



The reaction rate is given by the expression

$$\frac{d[C_xH_y]}{dt} = -B [C_xH_y]^a [O_2]^b e^{-E/RT}$$

Suggested values of B , E , a and b for various hydrocarbon fuels are given in the combustion literature.



Strengths of Finite Rate Chemistry

- Closer to real physics
- Expandable to many steps and many intermediate species
- Real species transport properties can be used
- Temperature-dependent reaction rates allow for consideration of flame extinction

Weaknesses of Finite Rate Chemistry

- Costly to track many different species and compute reaction rates
- Uncertainties in reaction parameters
- Only useful in DNS calculations where resolution fine enough to capture real molecular diffusion

Thermal Boundary Conditions

1. Adiabatic – No heat transfer through walls
2. Prescribed Temperature – Wall temperature is set by user
3. Thermally-Thin – Wall heats up according to its given density, specific heat and thickness δ

$$\delta \rho_s c_s \frac{dT_s}{dt} = \dot{q}_c'' + \dot{q}_r''$$

Individual values of ρ_s , c_s and δ not as important as their product. This product may be easier to determine experimentally rather than through measurements of each individual term.

4. Thermally-Thick – One-dimensional heat conduction equation is applied in the direction normal to the surface

$$\rho_s c_s \frac{\partial T_s}{\partial t} = k_s \frac{\partial^2 T_s}{\partial n^2} \quad ; \quad -k_s \frac{\partial T_s}{\partial n} \Big|_{\text{surface}} = \dot{q}_c'' + \dot{q}_r''$$

where ρ_s is the density, c_s the specific heat, and k_s the conductivity of the material. Assume wall has thickness δ . Divide wall up into N cells. Temperature in i th cell, $T_{s,i}$, updated in time with a Crank-Nicholson scheme

$$\frac{T_{s,i}^{n+1} - T_{s,i}^n}{\delta t_s} = \frac{\alpha}{2} \left(\frac{T_{s,i+1}^n - 2T_{s,i}^n + T_{s,i-1}^n}{\delta x_s^2} + \frac{T_{s,i+1}^{n+1} - 2T_{s,i}^{n+1} + T_{s,i-1}^{n+1}}{\delta x_s^2} \right)$$

where $\alpha = k/(\rho_s c_s)$ and $1 \leq i \leq N$. Boundary condition is discretized

$$-k_s \frac{T_{s,1} - T_{s,0}}{\delta x_s} = \dot{q}_c'' + \dot{q}_r'' - \dot{q}_e''$$

and wall temperature $T_w = (T_{s,0} + T_{s,1})/2$.

Convective Heat Flux

(DNS) \dot{q}_c'' directly obtained by differencing the gas phase temperature values in the cells adjacent to the boundary

$$\dot{q}_c'' = -k \frac{\partial T}{\partial n} \approx -k \frac{T_{in} - T_{gas}}{\delta n}$$

where n is the directional coordinate pointing into the wall and δn is the distance between cell centers

(LES) \dot{q}_c'' obtained from a correlation of the form

$$\dot{q}_c'' = -C |\Delta T|^{1/3} \Delta T \quad \text{W/m}^2$$

where $\Delta T = T_{wall} - T_{gas}$ is the difference between the gas and wall temperature, and C is an empirical constant of value 1.5 for a horizontal surface and 1.3 for a vertical surface.

Radiative Transport Equation

Radiative Transport Equation (RTE) for a non-scattering grey gas

$$\mathbf{s} \cdot \nabla I(\mathbf{x}, \mathbf{s}) = \kappa(\mathbf{x}) [I_b(\mathbf{x}) - I(\mathbf{x}, \mathbf{s})]$$

$I(\mathbf{x}, \mathbf{s})$	Radiant Intensity
$I_b(\mathbf{x})$	Radiant energy source term
\mathbf{s}	unit normal direction vector
$\kappa(\mathbf{x})$	Absorption Coefficient
σ	Stefan-Boltzmann Constant

Radiant heat flux vector \mathbf{q}_r defined

$$\mathbf{q}_r(\mathbf{x}) = \int \mathbf{s} I(\mathbf{x}, \mathbf{s}) d\mathbf{s}$$

Radiative loss term in the energy equation is

$$-\nabla \cdot \mathbf{q}_r(\mathbf{x}) = \kappa(\mathbf{x}) [U(\mathbf{x}) - 4\sigma T(\mathbf{x})^4] \quad ; \quad U(\mathbf{x}) = \int I(\mathbf{x}, \mathbf{s}) d\mathbf{s}$$

Net radiant energy flux gained by a grid cell is the difference between that which is absorbed and that which is emitted.

Source Terms

κ is the effective absorption coefficient assuming soot is the dominant absorber/emitter, with CO_2 , H_2O and Fuel playing smaller role. RadCal, a computer program designed to compute absorption coefficients for soot and various gases, generates a table for κ as a function of temperature and mixture fraction.

Source term must be modeled near flame because of lack of resolution.

$$\kappa I_b = \begin{cases} \kappa \sigma T^4 / \pi & \text{Outside flame zone} \\ \chi_r \dot{q}''' / 4\pi & \text{Inside flame zone} \end{cases} \quad (2)$$

Here, \dot{q}''' is the chemical heat release rate per unit volume and χ_r is the *local* fraction of that energy emitted as thermal radiation. Note the difference between the prescription of a local χ_r and the resulting global equivalent. For a small fire ($D < 1$ m), the local χ_r is approximately equal to its global counterpart. However, as the fire increases in size, the global value will typically decrease due to a net re-absorption of the thermal radiation by the increasing smoke mantle.

Flux Methods: Finite Volume, Discrete Ordinates, etc.

Return to original transport equation

$$\mathbf{s} \cdot \nabla I(\mathbf{x}, \mathbf{s}) = \kappa(\mathbf{x}) [I_b(\mathbf{x}) - I(\mathbf{x}, \mathbf{s})]$$

Integrate over grid cell ijk and an angle $\delta \mathbf{s}^l$, apply divergence theorem, and discretize:

$$\sum_{m=1}^6 A_m I_m^l (\mathbf{s}^l \cdot \mathbf{n}_m) \delta \mathbf{s}^l = \kappa_{ijk} [I_{b,ijk} - I_{ijk}^l] V_{ijk} \delta \mathbf{s}^l$$

I_{ijk}^l	Radiant Intensity in direction l
I_m^l	Radiant Intensity at cell face m
$I_{b,ijk}$	Radiant source term
$\delta \mathbf{s}^l$	Solid angle corresponding to direction l
V_{ijk}	Volume of cell ijk
A_m	Area of cell face m

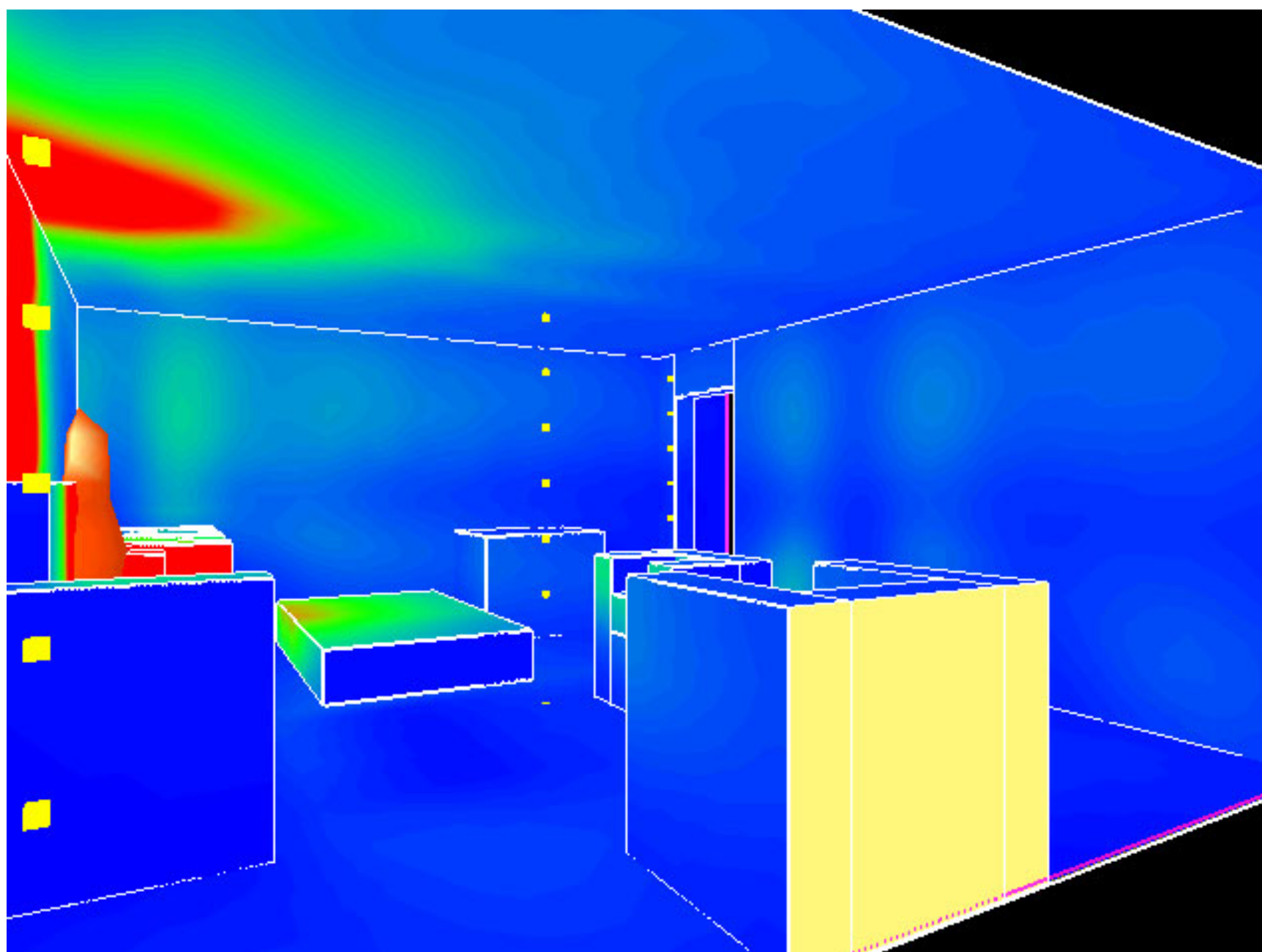
Reference: Kim and Huh, "Assessment of the Finite Volume Method...", *Numerical Heat Transfer, Part B*, **35**:85–112 (1999).

Strengths of Finite Volume Method

- Closer to real physics; less approximation
- Good in optically-thin limit

Weaknesses of Finite Volume Method

- Requires discretization over many angles to rid grid/angular dependency
- Can be expensive



Heat of Vaporization

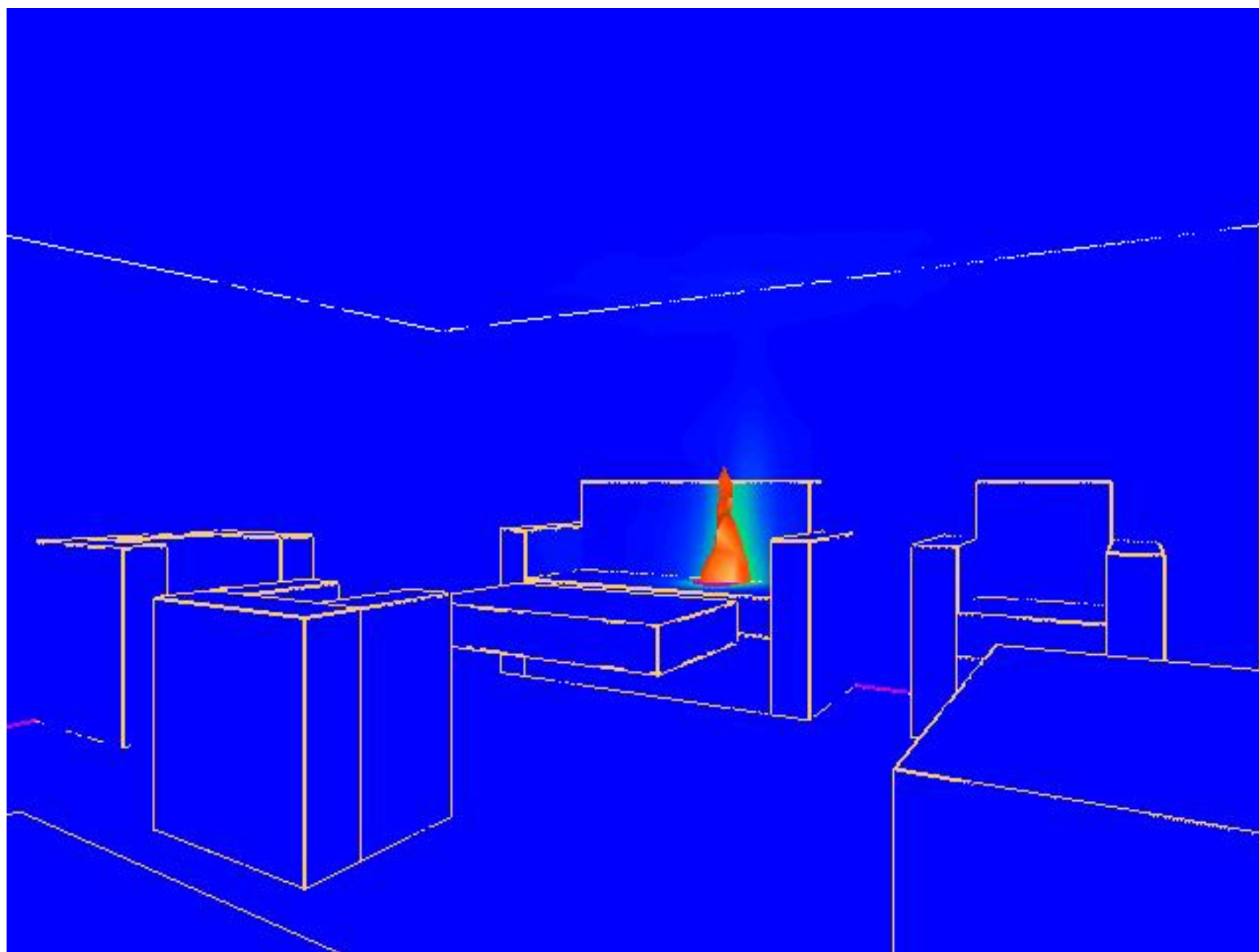
Mass burning rate per unit area approximately given by

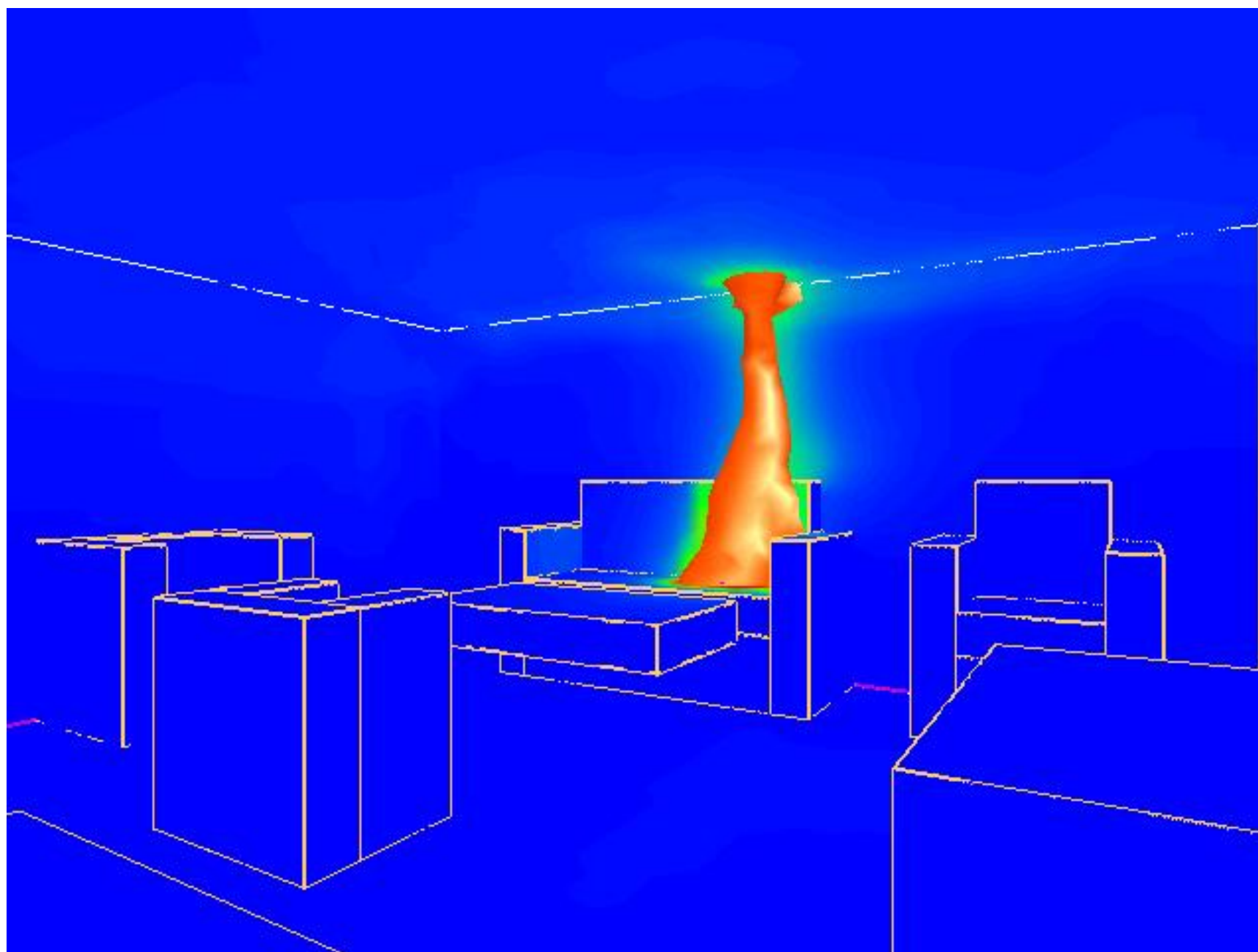
$$\dot{m}'' = \frac{\dot{q}_{net}''}{L}$$

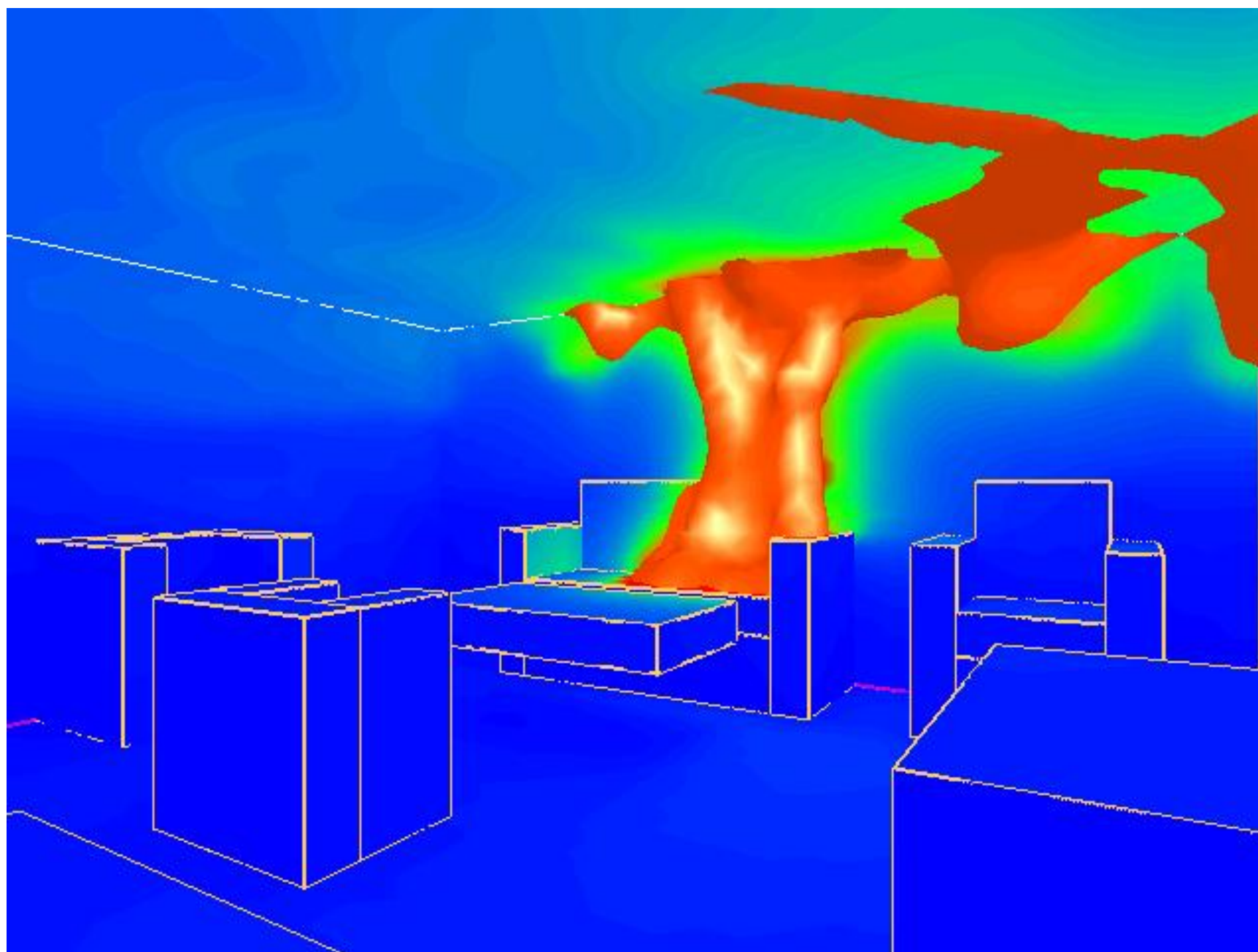
where \dot{q}_{net}'' is the net heat flux into the fuel and L is the Heat of Vaporization.

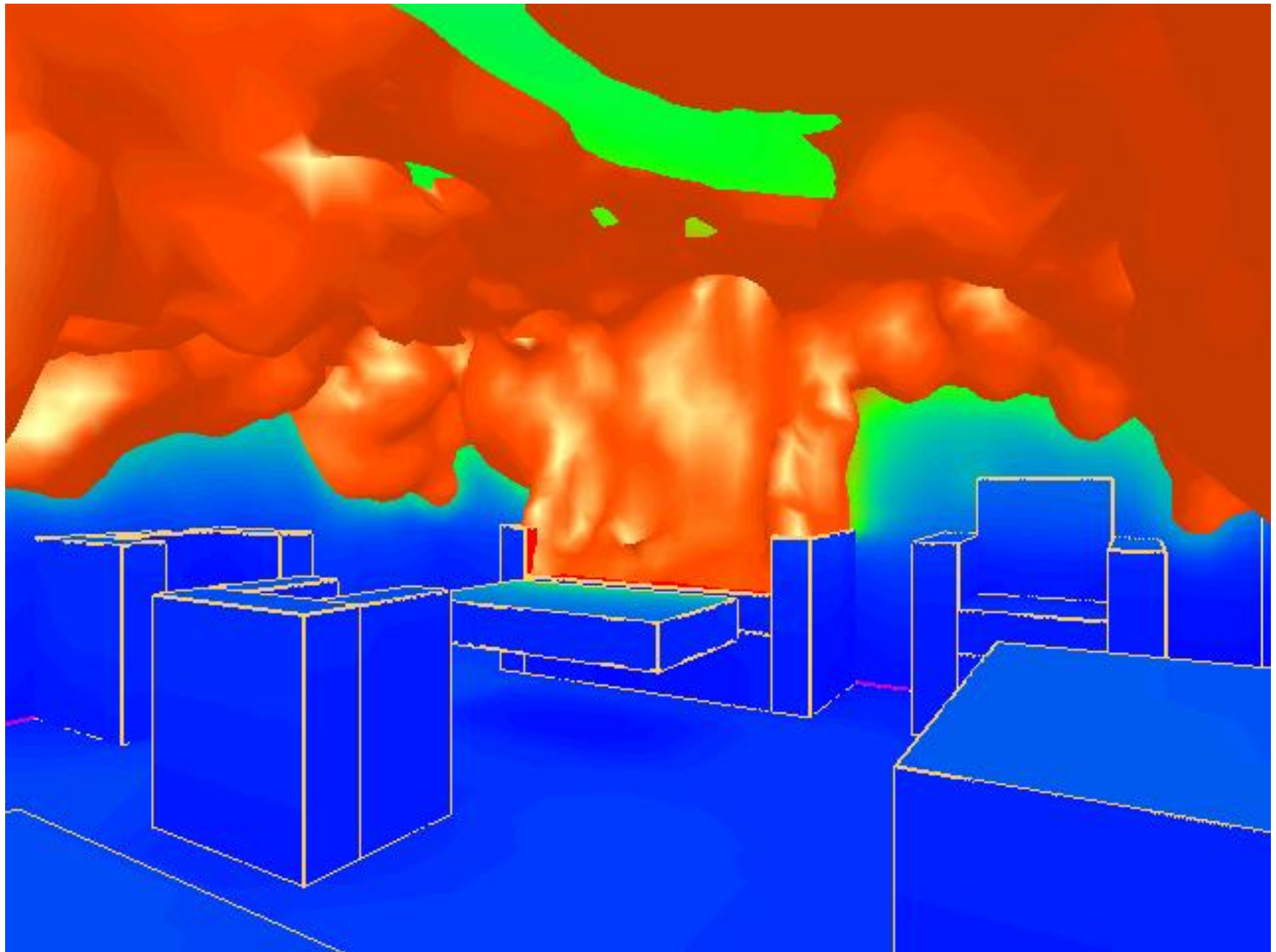
Quintiere's "Principles of Fire Behavior" suggests

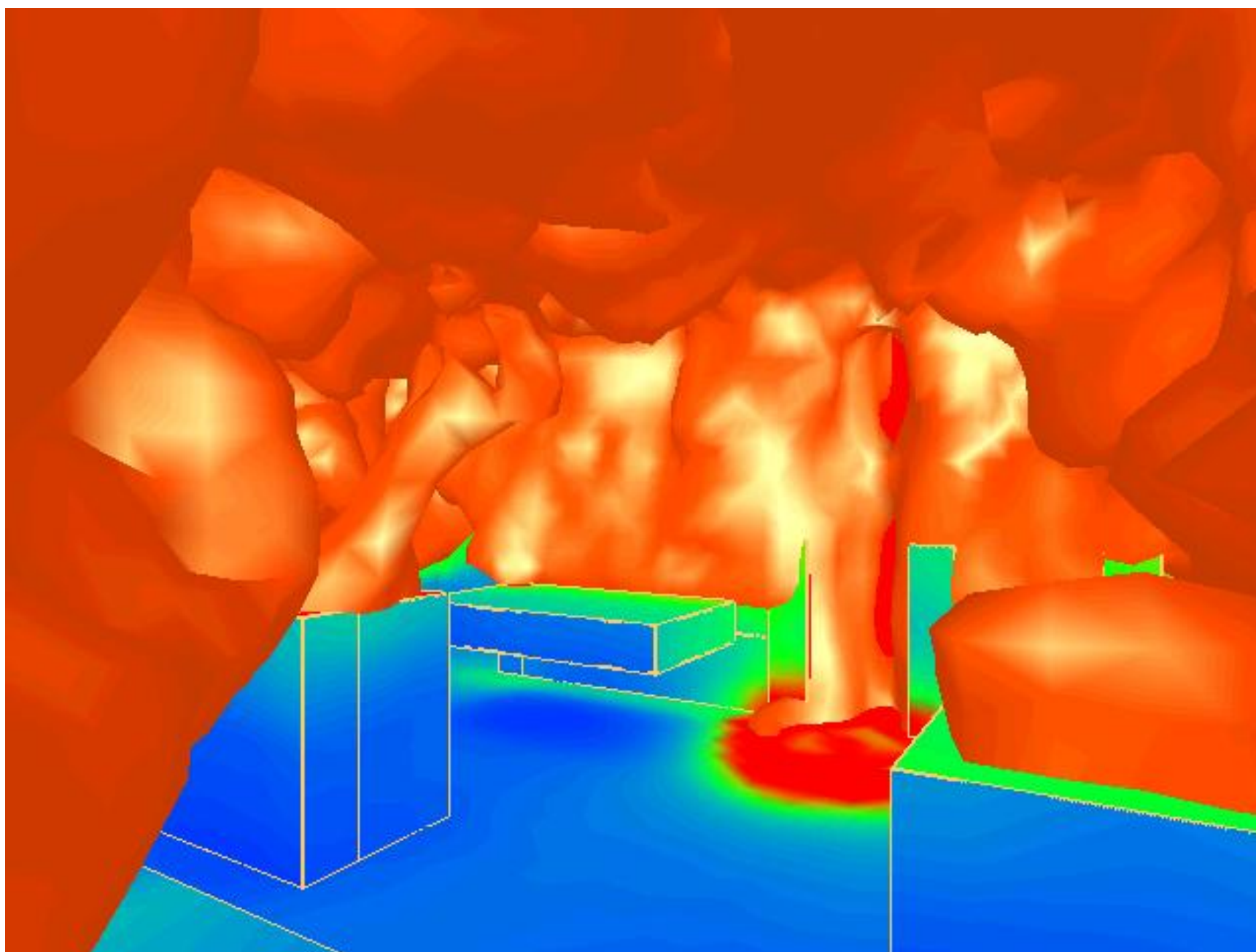
Liquids	< 1000 kJ/kg
Thermoplastics	1000 – 3000 kJ/kg
Char Formers	2000 – 6000 kJ/kg











Prescribing Thermal Boundary Conditions

Thermally-thick solid:

- Thermal Diffusivity, $\alpha = k/(\rho c)$, ALPHA (m²/s)
- Thermal Conductivity, k , KS (W/m·K)
- Thickness, δ DELTA (m)

Thermally-thin sheet:

- Thermal Capacitance, $c\delta\rho$ C_DELTA_RHO, (kJ/kg-K \times m \times kg/m³=kJ/m²/K)

For either Thermally-thick or thin, one can set

- EMISSIVITY, 1 by default.
- TMPIGN, ignition temperature (C)
- BACKING= ' INSULATED ' , no heat transfer off the back side of the surface liner.

Prescribing the Fire

HRRPUA Heat Release Rate Per Unit Area (kW/m^2).

HEAT_OF_VAPORIZATION (kJ/kg). This is an alternative to HRRPUA. This is the amount of energy required to vaporize a solid or liquid fuel once it has reached its ignition temperature `TMPIGN`. If it is desired that the burning rate of the fuel be dependent on heat feedback from the fire, use this parameter rather than HRRPUA.

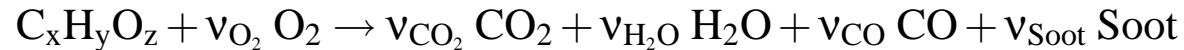
DENSITY **or** SURFACE_DENSITY The density (kg/m^3) or surface density (kg/m^2) of the fuel. This parameter is only needed if it is desired that the fuel eventually burn away. Only one of these parameters ought to be prescribed. If neither is prescribed, the fuel will never be exhausted. Note that if SURFACE_DENSITY is prescribed, when the fuel is exhausted, the underlying solid will remain intact, whereas if DENSITY is prescribed, the underlying solid will be removed from the calculation.

HEAT_OF_COMBUSTION (kJ/kg) Optional parameter that is needed only if a HEAT_OF_VAPORIZATION has been specified and the heat of combustion of the material differs from that specified by the governing REACTION.

Following are a few examples of SURF lines. These and several others are found in the DATABASE file.

```
&SURF ID          = 'CONCRETE'
      FYI          = 'Thermally-thick material'
      ALPHA        = 5.7E-7
      KS           = 1.0
      DELTA        = 0.2 /
&SURF ID          = 'UPHOLSTERY'
      FYI          = 'Fleischmann and Chen, 100% acrylic'
      C_DELTA_RHO  = 1.29
      BACKING      = 'INSULATED'
      TMPIGN       = 280.
      DENSITY      = 20.0
      HEAT_OF_VAPORIZATION=2500. /
&SURF ID          = 'SHEET METAL'
      FYI          = 'Thermally-thin material'
      C_DELTA_RHO  = 4.7 /
```

Prescribing REACtion Parameters



ID A character string naming the reaction.

NU_O2, NU_H2O, NU_FUEL, NU_CO2 Ideal stoichiometric coefficients for the reaction of a hydrocarbon fuel. Default: propane.

MW_FUEL Molecular weight of the fuel (g/mol).

SOOT_YIELD The fraction of fuel mass converted into smoke particulate.

CO_YIELD The fraction of fuel mass converted into carbon monoxide. Normally, this parameter need not be set, because by default, the CO_YIELD, y_{CO} , is linked to the SOOT_YIELD, y_s , via the correlation (Köylü and Faeth)

$$y_{CO} = \frac{M_{Cx}}{M_f \nu_f} 0.0014 + 0.37 y_s$$

EPUMO2 Energy Per Unit Mass Oxygen, ΔH_{O_2} (kJ/kg). The amount of energy released per unit mass of oxygen consumed. (Default 13,100 kJ/kg). Note that the heat of combustion is assumed to be

$$\Delta H = \frac{\nu_{O_2} M_{O_2}}{\nu_f M_f} \Delta H_{O_2}$$

RADIATIVE_FRACTION The fraction of energy released from the flame as thermal radiation. Recall source term in Radiation Transport Equation:

$$\kappa I_b = \begin{cases} \kappa \sigma T^4 / \pi & \text{Outside flame zone} \\ \chi_r \dot{q}''' / 4\pi & \text{Inside flame zone} \end{cases}$$

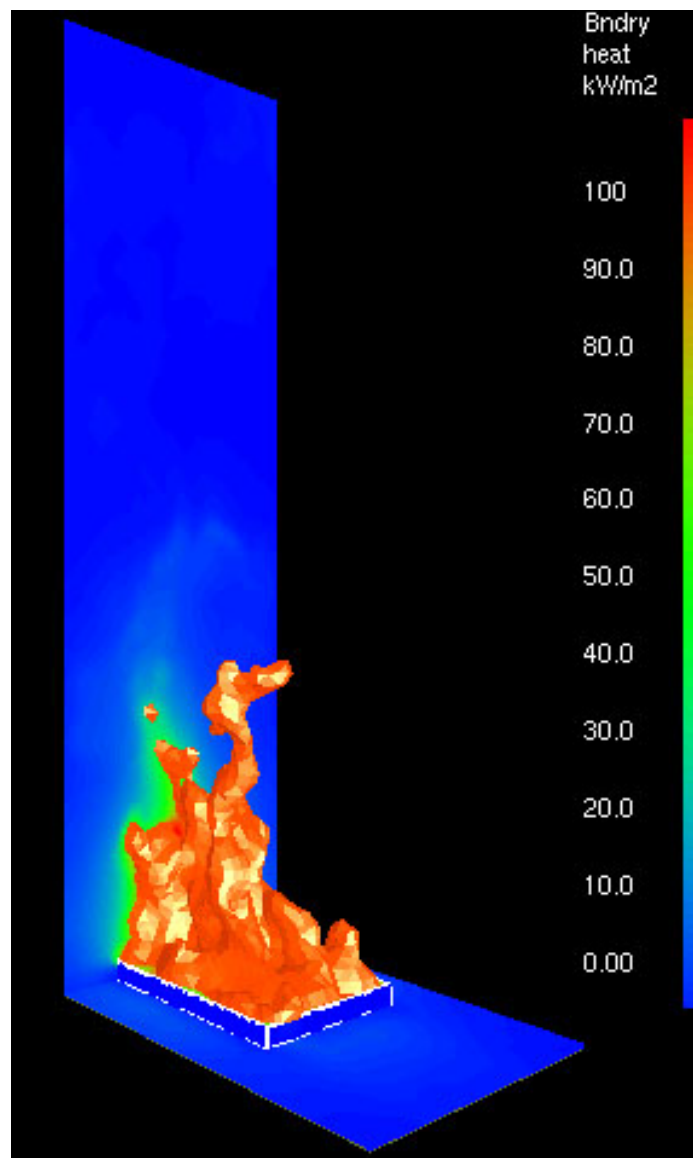
A few sample REAC lines are given here. More can be found in the DATABASE file.

```
&REAC ID= 'METHANE'
      MW_FUEL=16
      NU_O2=2.
      NU_CO2=1.
      NU_H2O=2.
      RADIATIVE_FRACTION=0.15
      SOOT_YIELD=0.01 /
```

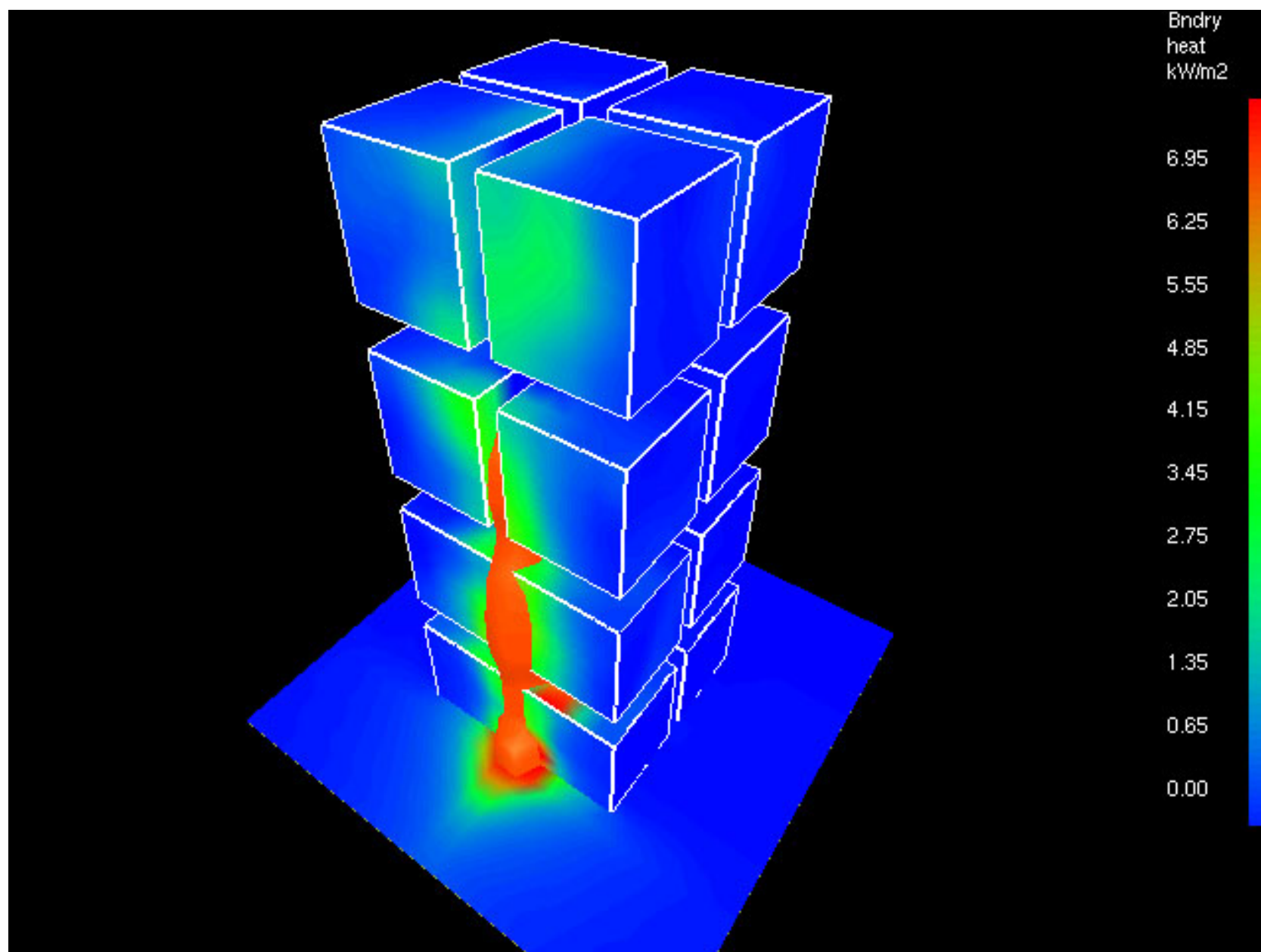
```
&REAC ID= 'WOOD'
      SOOT_YIELD = 0.01
      NU_O2      = 3.7
      NU_CO2     = 3.4
      NU_H2O     = 3.1
      MW_FUEL    = 87.
      EPUMO2     = 8850. /
```

Flame Spread Example

```
&HEAD CHID='wall',TITLE='Wall Fire' /
&GRID IBAR=20,JBAR=5,KBAR=20 /
&PDIM XBAR0=-1.00,XBAR=1.00,YBAR0=0.00,YBAR=0.50,ZBAR=2.00 /
&TIME TWFIN=60. /
&SURF ID='burner',HRRPUA=676. /
&SURF ID='WALL',C_DELTA_RHO=0.80,TMPIGN=200.,HRRPUA=300. /
&OBST XB=-.14,0.14,0.00,0.28,0.00,0.03,SURF_IDS='burner','INERT','INERT'
&VENT CB='XBAR',SURF_ID='OPEN' /
&VENT CB='XBAR0',SURF_ID='OPEN' /
&VENT CB='YBAR',SURF_ID='OPEN' /
&VENT CB='YBAR0',SURF_ID='WALL' /
&VENT CB='ZBAR',SURF_ID='OPEN' /
&BNDF QUANTITY='RADIATIVE_FLUX' /
&BNDF QUANTITY='CONVECTIVE_FLUX' /
&BNDF QUANTITY='BURNING_RATE' /
&BNDF QUANTITY='WALL_TEMPERATURE' /
```

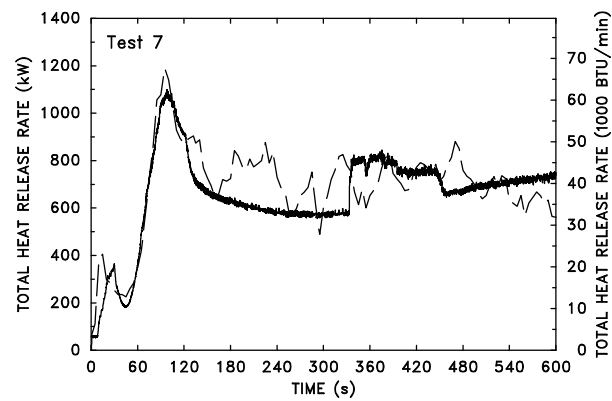
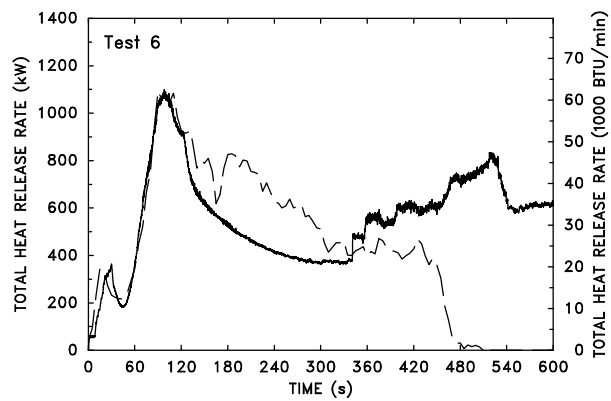
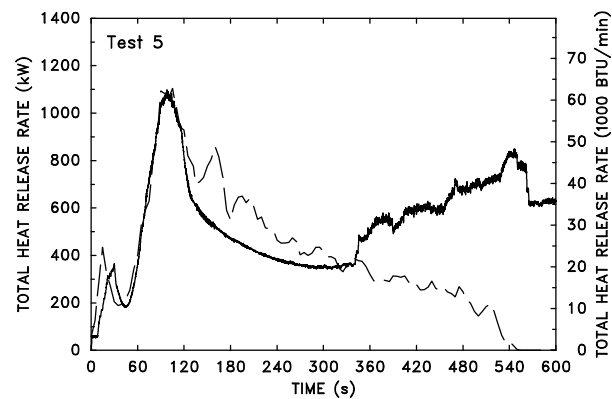
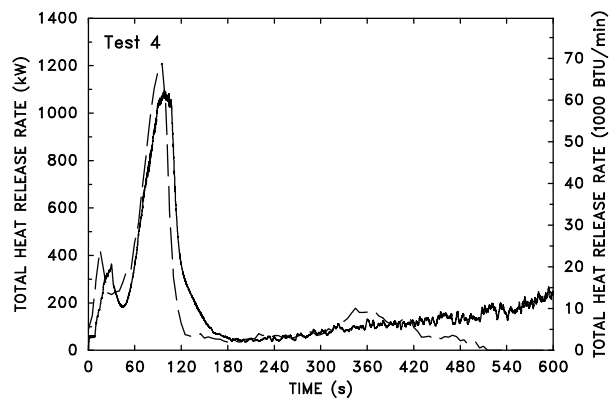
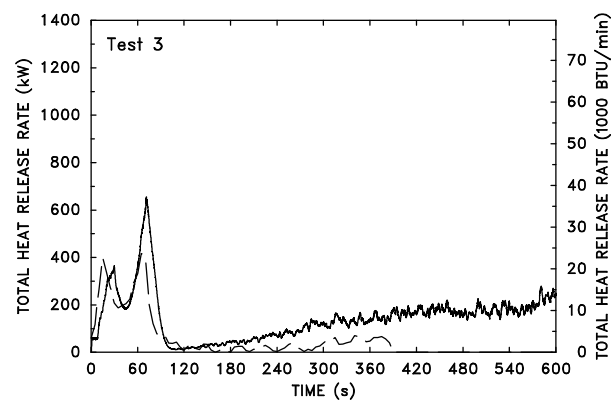
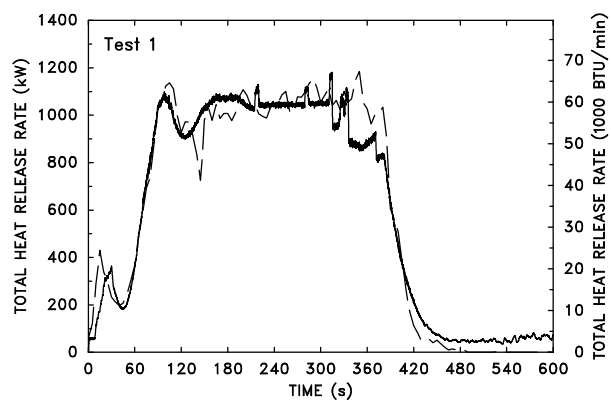


Example: Burning Boxes



```
&SURF ID                      = 'PLASTIC A'
      HRRPUA                  = 420.
      RAMP_Q                  = 'GAP'
      C_DELTA_RHO             = 1.0
      TMPIGN                   = 370. /
&RAMP ID='GAP',T= 0.0,F=0.0 /
&RAMP ID='GAP',T= 1.0,F=0.6 /
&RAMP ID='GAP',T= 30.0,F=0.2 /
&RAMP ID='GAP',T= 80.0,F=1.6 /
&RAMP ID='GAP',T= 100.0,F=1.0 /
```





Sprinkler Activation

Link temperature estimated from the differential equation

$$\frac{dT_l}{dt} = \frac{\sqrt{|\mathbf{u}|}}{\text{RTI}} (T_g - T_l) - \frac{C}{\text{RTI}} (T_l - T_m) - \frac{C_2}{\text{RTI}} \beta |\mathbf{u}|$$

T_l	link temperature
T_g	gas temperature near link
T_m	mount temperature (usually assumed ambient)
$ \mathbf{u} $	gas speed near link
RTI	Response Time Index
C	Conduction or “C-Factor”
C_2	water cooling coefficient
β	water volume fraction

Droplet Sizes

Once activation is predicted, a sampled set of water droplets are tracked from the sprinkler to either the floor or the burning commodity. In order to compute the droplet trajectories, the initial size and velocity of each droplet must be prescribed. This is done in terms of random distributions. The initial droplet size distribution of the sprinkler spray is expressed in terms of its Cumulative Volume Fraction (CVF). For droplets, Chan at FM suggests a combination of the Rosin-Rammler distribution with a log-normal distribution

$$F(d) = \begin{cases} \frac{1}{\sqrt{2\pi}} \int_0^d \frac{1}{\sigma d'} e^{-\frac{[\ln(d'/d_m)]^2}{2\sigma^2}} dd' & (d \leq d_m) \\ 1 - e^{-0.693\left(\frac{d}{d_m}\right)^\gamma} & (d_m < d) \end{cases}$$

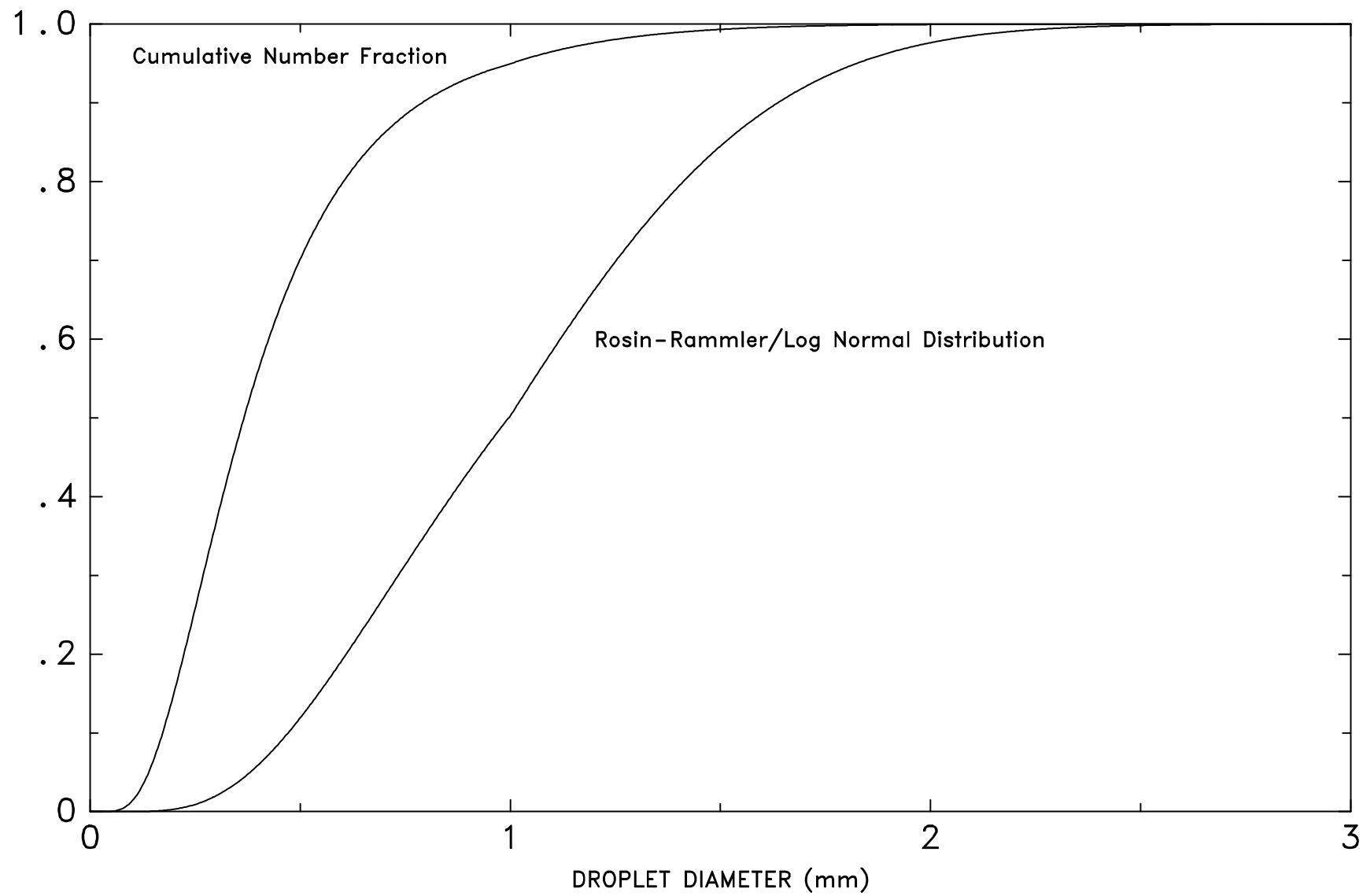
where d_m is the median droplet diameter (*i.e.* half the mass is carried by droplets d_m or smaller in diameter), and γ and σ are empirical constants equal to about 2.4 and 0.58, respectively.

A Probability Density Function (PDF) for the droplet diameter is defined

$$f(d) = \frac{F'(d)}{d^3} \bigg/ \int_0^\infty \frac{F'(d')}{d'^3} dd'$$

Droplet diameters are randomly selected by equating the Cumulative Number Fraction of the droplet distribution with a uniformly distributed random variable U

$$U(d) = \int_0^d f(d') dd'$$



Droplet Trajectory

External force term \mathbf{f} in the momentum equation is

$$\mathbf{f} = \frac{1}{2} \frac{\sum \rho C_d A_d (\mathbf{u} - \mathbf{u}_d) |\mathbf{u} - \mathbf{u}_d|}{V}$$

C_d	Drag Coefficient
A_d	Cross sectional area of the droplet
\mathbf{u}	Gas velocity
\mathbf{u}_d	Droplet velocity
V	Volume of grid cell

$$C_D = \begin{cases} 24/\text{Re} & \text{Re} < 1 \\ 24 \left(1 + 0.15 \text{Re}^{0.687} \right) / \text{Re} & 1 < \text{Re} < 1000 \\ 0.44 & 1000 < \text{Re} \end{cases}$$

$$\text{Re} = \frac{\rho |\mathbf{u}_d - \mathbf{u}| 2r_d}{\mu}$$

Droplet trajectory governed by

$$\frac{d}{dt}(m_d \mathbf{u}_d) = m_d \mathbf{g} - \frac{1}{2} \rho C_d A_d (\mathbf{u} - \mathbf{u}_d) |\mathbf{u} - \mathbf{u}_d|$$

where m_d is the mass of the droplet.

When a water droplet hits a solid horizontal surface, it is assigned a random horizontal direction and moves at a fixed velocity until it reaches the edge, at which point it drops straight down at a constant speed. This terminal velocity has been measured to be roughly 0.5 m/s.

Droplet Evaporation

Mass loss rate of droplet given by empirical relation

$$\frac{dm_d}{dt} = -2\pi r_d \text{Sh } \rho D (Y_d - Y_g)$$

m_d	Mass of a droplet
r_d	Radius of a droplet
ρ	Density of air
D	Diffusivity of water vapor into air
Sh	Sherwood number $\text{Sh} = 2 + 0.6 \text{Re}^{\frac{1}{2}} \text{Sc}^{\frac{1}{3}}$
Re	Reynolds number based on droplet velocity and drop diameter
Sc	Schmidt number
Y_d	Mass fraction of water vapor at droplet surface
Y_g	Mass fraction of water vapor in the air

Mole fraction of water vapor at droplet surface given by Clausius-Clapeyron equation

$$X_d = \exp \left[\frac{h_v M_w}{\mathcal{R}} \left(\frac{1}{T_b} - \frac{1}{T_d} \right) \right] \quad ; \quad Y_d = \frac{X_d}{X_d(1 - M_a/M_w) + M_a/M_w}$$

X_d	Mole fraction of water vapor at droplet surface
T_d	Droplet temperature
T_b	Water boiling temperature
h_v	Heat of vaporization of water
M_w	Molecular weight of water vapor
M_a	Molecular weight of air
\mathcal{R}	Gas constant

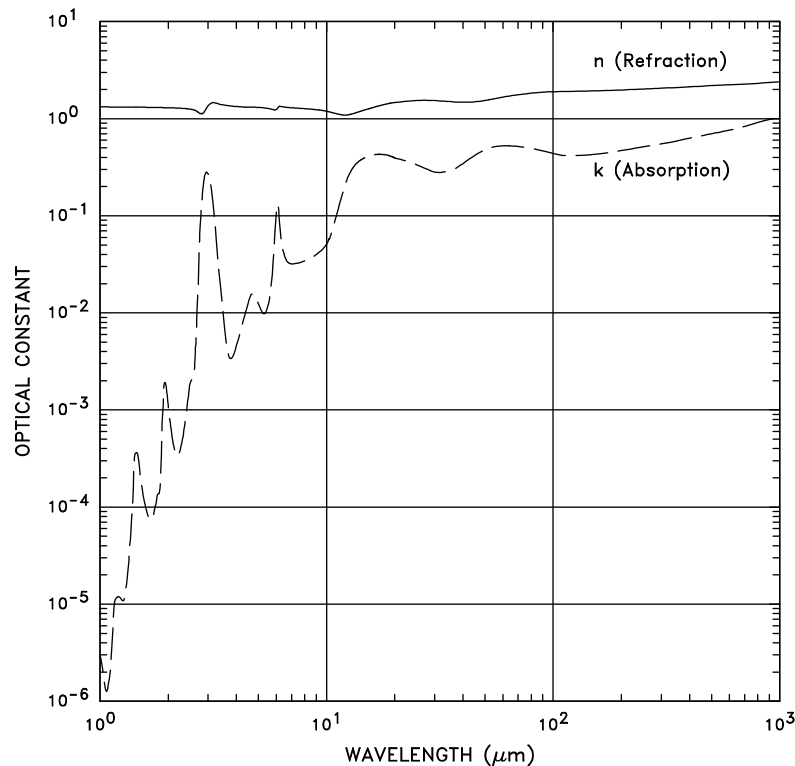
Energy balance for droplet

$$m_d c_w \frac{dT_d}{dt} = A_d h_d (T_g - T_d) - \frac{dm_d}{dt} h_v$$

c_w	Specific heat of water
T_g	Gas temperature
h_d	Heat transfer coefficient, $\text{Nu } k_a / 2r_d$
Nu	Nusselt number, $2 + 0.6 \text{Re}^{1/2} \text{Pr}^{1/3}$
Pr	Prandtl number of air (0.7)
k_a	Thermal conductivity of air
A_d	Surface area of droplet

Radiation Absorption

The attenuation of thermal radiation by water droplets especially important for water mist systems. Water droplets attenuate thermal radiation through a combination of scattering and absorption, typically represented by a wavelength dependent complex number, $n + ik$, called the refractive index. In this expression n is the refractive factor of the index, used in Snell's Law to determine the bending of light at a material interface, and k is the extinction coefficient.



Simplified theory approximates scattering and absorption processes as a function of the droplet size and liquid water concentration in the hot gas:

$$\frac{I}{I_0} = e^{-3KW L/4r_d \rho_w}$$

I_0	incoming radiant intensity
I	outgoing radiant intensity
K	wavelength-averaged, radius-dependent extinction coefficient
W	water mass per unit volume gas
L	pathlength
r_d	droplet radius
ρ_w	density of water

An extinction coefficient K is calculated as a function of droplet radius. K is the sum of scattering, K_s , and absorption, K_a , coefficients, integrated over the wavelengths of interest:

$$K_s(\lambda, r_d) = 2 \left[1 + \frac{1}{\alpha(n-1)} \left(1 - \frac{\cos(2\alpha(n-1))}{2\alpha(n-1)} - \sin(2\alpha(n-1)) \right) \right]$$

$$K_a(\lambda, r_d) = 1 + \frac{2(\exp(-4\alpha nk) + (\exp(-4\alpha nk) - 1)/(4\alpha nk))}{4\alpha nk} \quad ; \quad \alpha = \frac{2\pi r_d}{\lambda}$$

Extinguishment

Extinguishment of the fire is the single most difficult component of the numerical model. To date, most of the work in this area has been performed at Factory Mutual. An analysis by Yu yields an expression for the total heat release rate from a rack storage fire after sprinkler activation

$$\dot{Q} = \dot{Q}_0 e^{-k(t-t_0)}$$

where \dot{Q}_0 is the total heat release rate at the time of application t_0 , and k is a fuel-dependent constant that for the FMRC Standard Plastic commodity is given as

$$k = 0.176 \dot{m}_w'' - 0.0131 \quad \text{s}^{-1}$$

The quantity \dot{m}_w'' is the flow rate of water impinging on the box tops, divided by the area of exposed surface (top and sides). It is expressed in units of kg/m²/s.

Locally, it is assumed

$$\dot{q}_f''(t) = \dot{q}_{f,0}''(t) e^{-\int k(t) dt}$$

$\dot{q}_{f,0}''(t)$	Heat Release Rate Per Unit Area (no water)
$k(t)$	$a \dot{m}_w'' \text{ s}^{-1}$
\dot{m}_w''	Water Mass Per Unit Area (kg/m ²)

Sprinkler Implementation (FDS v2)

Sprinklers are invoked in the input file with a line:

```
&MISC ... ,DATABASE_DIRECTORY='c:\nist\fds\database2\' /  
      .  
      .  
      .  
&SPRK XYZ=2.6,4.3,1.5,MAKE='Splash-2000' /
```

where `Splash-2000` is the name of a particular sprinkler whose activation and spray characteristics are contained in a separate file. Usually this file is stored in the same directory as the `database2.data` file.

Sprinkler data file (for example `Splash-2000.spk`) has the following format:

MANUFACTURER

Acme

MODEL

Splash-2000

OPERATING_PRESSURE

0.48

K-FACTOR

79.

RTI

110.

C-FACTOR

0.

ACTIVATION_TEMPERATURE

74.

OFFSET_DISTANCE

0.20

SIZE_DISTRIBUTION

1

800 2.43 0.6

VELOCITY

2

61,36

6.3,6.4,6.5,6.8,6.8,6.8,6.8,6.8,6.8,6.8,6.8,6.8,6.5,6.4,...

.

.

FLUX

2

61,36

11.9,13.0,13.5,16.4,16.4,16.4,16.4,16.4,16.4,16.4,16.4,16.4,...

.

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